4th INTERNATIONAL CONFERENCE ON THERMAL PROCESS MODELING AND COMPUTER SIMULATION

31 May – 2 June 2010 Shanghai, CHINA

CONFERENCE PROGRAM
&
ABSTRACT BOOK

Contents

FORWARD

Welcome to ICTPMCS-2010!

This is the 4th INTERNATIONAL CONFERENCE ON THERMAL PROCESS MODELING AND COMPUTER SIMULATION (ICTPMCS-2010). The conference is for the second time held in Shanghai, China. It is a great honor for Shanghai Jiao Tong University (SJTU) to organize the event again.

Due to increasingly powerful computers and advanced mathematical tools, the materials community finds itself on the verge of another revolution. Scientists and engineers can now guide advanced materials/processes development based on simulation. They are also able to understand how materials behave under changing conditions, and how processes can improve materials performance. Totally 177 papers in oral and poster respectively, including invited 8 plenary and 14 keynote lectures will be presented at the conference. It is believed that these papers have represented the developments in the field of modeling and computer simulation of thermal processes in current status, and will also offer a guideline for all participants.

The participants can have the opportunity for progressive discussing and exchanging the state-of-the-art information and their views in the simulation technology in thermal processes and related materials research field. We would like to gratefully express our appreciation to those who contribute to the success of this conference.

We wish you the stimulating and interesting conference participation as well as enjoyable stay in Shanghai.

May 2010

Co-Chairmen of ICTPMCS-2010

Dr. George E. Totten
Texas A&M University

Prof. Weimin Zhang
Shanghai Jiao Tong University

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Conference Sponsors

International Federation for Heat Treatment and Surface Engineering

Shanghai Jiao Tong University

Chinese Heat Treatment Society

GENERAL INFORMATION

Period

31 May – 02 June 2010

Venue

Shanghai Sheshan Forest Hotel
Songjiang, Shanghai 201602
Tel.: +86-21-57651160
Fax: +86-21-57651169
http://www.sh-foresthotel.com/

Language

English

Conference Website

http://www.ictpmcs2010.sjtu.edu.cn/

SOCIAL EVENTS

Reception Buffet, 30 May (Sunday) 2010 18:30 – 20:30, Sunshine Dining Hall, Sheshan Forest Hotel
Visiting World EXPO 2010, 02 June (Wednesday) 2010, Shanghai
Banquet, 01June (Tuesday) 2010 18:30 – 20:30, Sunshine Dining Hall, Sheshan Forest Hotel

ACCOMMODATION

- **Sheshan Forest Hotel** (Venue)
  Address: 9289 Waiqingsong Road, Songjiang District, Shanghai, P.C.201602
  Tel: +86-21-5765160
  Service: Breakfast, Free Wireless Internet Access in Room
- **Lansun Mountain Villa** (5 minutes walk to the venue)
  Address: 9269 Waiqingsong Road, Songjiang District, Shanghai, P.C.201602
  Tel: +86-21-57651170
  Service: Breakfast, Internet Access by Cable in Room

GUIDELINE FOR PRESENTATIONS

ORAL SESSION PRESENTATION

Except the invited plenary and keynote speakers, 15 min talk + 5 min discussion per each

- The session-chairs are requested to meet speakers of their sessions in the allotted session rooms at least 15 minutes prior to the commencement of the session. If the session chair(s) can not chair the allotted session, please contact the Conference Secretariat one day prior to the session.
- The oral-presenting authors should show up at the allotted session room 15 minutes earlier before the session starts. Pre-view and copying of the oral presentation documents can be made in the related session room in advance. The individual session program for the current day will be shown at the entrance of each session room and the Notice Board, if any modification is being made.
- Multi-media projector is available for oral presentation.

POSTER SESSION PRESENTATION

- Poster presenting authors are requested to carefully prepare their posters fit into maximum dimensions 120 cm (height) and 100 cm (width), the paper ID number should be obviously showed at the **top left corner** of the poster. Simply enlarged abstract or manuscript of the paper is not suitable to appear!
- The authors should stick the poster on the board after plenary session on 31 May by using nails and/or tape provided by the conference at the site. The authors should show up during the poster session period and remove his/her poster after the presentation ends.

PUBLICATION OF SUBMITTED PAPERS

Each registered participant allows submitting max one paper only for presentation at the conference and later for publication. The maximum pages would be 4 pages A4 for contributed papers and 6 pages for invited papers. Please prepare your final manuscripts according to the proceedings paper instructions (see 2nd Circular). And please submit the final full-length text of the manuscript to the Secretariat of ICTPMCS via Email directly by 30 April 2010.

All submitted papers have the chance to be, respectively, recruited and published in one of the following journals:

- Materials Science and Technology (SCI)
- International Heat Treatment and Surface Engineering (IFHTSE official journal, EI)
- Journal of Shanghai Jiao Tong University (EI)

after strict quality control by peer review organized by a special panel but the relevant journal's editors keep the right of final decision on acceptance.

The authors of accepted papers **have to pay the publication fee** afterwards. The amount of the payment depends on the regulation of the journal who accepts to publishing.

CONFERENCE PROGRAM

30 May (SUN)	09:00 – 22:00	*Registering* at *lobby of Forest Hotel*				
	Evening	*Reception Buffet*				
31 May (MON)	08:00 – 08:40	Opening Ceremony at *Ballroom*				
	08:40 – 09:50	Plenary Session A(a) at *Ballroom*				
		Coffee Break				
	10:20 – 12:05	Plenary Session A(b) at *Ballroom*				
		Lunch				
	13:00 – 14:45	Plenary Session A(c) at *Ballroom*				
Meeting Room No.		1	4	3	2	5
31 May (MON)	15:15 – 17:00	B(a)	C(a)	D(a)	E(a)	G(a)
		Supper				
	18:30 – 21:30	Poster Sessions at *Ballroom*				
01 June (TUE)	08:00 - 10:00	B(b)	C(b)	D(b)	E(b)	G(b)
		Coffee Break				
	10:30 – 12:00	B(c)	C(c)	D(c)	E(c)	G(c)
		Lunch				
	13:00 – 15:00	B(d)	C(c)	D(d)	F(a)	F(b)
		Coffee Break				
	15:30 – 17:30	H(a)	H(b)	D(e)	H(c)	F(c)
	Evening	*Conference Banquet*				
02 June (WED)	Whole day	*Visiting World Expo 2010*				
03 June (THU)		*Checking out*				
ICTPMCS-2010 Secretariat at Building 5-5101						

TOPICS OF SESSION

A – Plenary Session
B – Phase transformation & Alloy design
C – Heat treatment
D – Deformation & Recrystallization
E – Residual stress & Distortion
F – Melting & Casting
G – Welding & Coating
H – Miscellaneous

MAP OF MEETING ROOMS

Date & Time	Ballroom
31 MAY (MON)	**OPENING CEREMONY & PLENARY SESSIONS**
08:00 - 08:40	**Opening Ceremony Chair: *Prof. Weimin ZHANG***
	Prof. Wenjun ZHANG (*SJTU* President) **Dr George E Totten (*Conference Chair*)** **Dr Robert B Wood (*IFHTSE Secretary General*)**
08:40 - 09:50	**Plenary Session A(a) Chair: *Prof. Evan MA***
	A1 George E Totten *Process modeling for heat treatment: Current status and future developments* **A2 T Inoue** *A Mechanism of transformation plasticity and the identification of the characteristics*
09:50 - 10:20	***Coffee Break***
10:20 - 12:05	**Plenary Session A(b) Chair: *Prof. T Inoue***
	A4 Jianguo LIN *Hybrid forming processes for the production of lightweight high-strength automotive panel parts* **A7 Jian LU** *Integrated design of product and component realized by thermal processes with pre-stressed engineering approach* **A5 S Denis** *Prediction of heat treatment residual stresses and distortions: Recent developments*
12:05 - 13:00	***Lunch***
13:00 - 14:45	**Plenary Session A(c) Chair: *Prof. Jian LU***
	A6 Baicheng LIU *Modeling and simulation on deformation of heavy hydro turbine castings during casting and heat treatment processes* **A3 Jiansheng PAN** *Green heat treatment – the sustainable way of industrial developments* **A8 Evan MA** *Modeling amorphous structures produced by melt quenching: Zr-Cu-Al bulk metallic glass versus Ge-Sb-Te chalcogenide phase-change glass*
14:45 - 15:15	***Coffee Break***

Date & Time	Room No. 1	Room No. 4	Room No. 3	Room No. 2	Room No. 5
31 MAY (MON)	**PARALLEL SESSIONS - 1**				
15:15 - 17:00	**Session B(a)** **Chairs:** ***Profs. Xuejun JIN & Huiping LI***	**Session C(a)** **Chairs:** ***Profs. S MacKenzie & D Landek***	**Session D(a)** **Chairs:** ***Profs. Jianguo LIN & A Gontarz***	**Session E(a)** **Chairs:** ***Profs. Liu-Ho CHIU & T Luebben***	**Session G(a)** **Chairs:** ***Profs. Hao LU & Bolin HE***
	B13 **Bo WU** **B12** Chaoyang SUN **B03** Zhuo YU **B10** Gangbo TANG **D11** Jun DING	**E04** **BL Ferguson** **C09** Zhichao LI **C10** K Cvetkovski **C01** Weimin GAO **C14** Tao CONG	**D01** A Gontarz **D02** Z Pater **D03** Haibo XIE **D04** Xiawei YANG **D07** Jixiang ZHANG	**E01** **Young-Kook LEE** **E06** S Mackenzie **E09** Dae-Hoon KO **E02** T Luebben **E03** J Rath	**G13** **Hsin-Chih LIN** **G06** Yongcheng LIN **G07** Jihong YANG **G11** Changwen CUI **G09** Zhenhai XU
17:00 - 18:00	***Supper***				
Date & Time	**Room No. 1**				
31 MAY (MON)	**POSTER SESSIONS**				
18:30 - 21:30	**b09** Jing WU **b11** Naqiong ZHU **b16** Xiangying MENG **b26** Shikun XIE **b27** Shanglei YANG **b28** Hong DING **b30** Ping DONG **b33** Ning YU	**c15** H Yahagi **c19** Huiping LI **c21** Xunwei ZUO **c22** Yingli ZHAO **c23** Dongying JU	**d10** Xiangru LIU **d15** Ben ZENG **d17** Lin CHEN **d27** Guanyu DENG **d29** Shu GUO **d30** Junqing GUO **d31** Xiaochun MA **d32** Junguang HE **d33** Lei ZHANG **d34** Yu ZHANG **d39** Bin TANG **d42** Yongge FANG	**f11** Yitao YANG **f15** Zhijun YANG **g04** Yansong ZHANG **g08** A Sliwa **g14** Yong SUN **g15** Bolin HE **g16** Wenya LI **g17** Yong HU **g18** Zhi ZHANG	**h08** Yinghua JIANG **h21** Yusen YANG **h22** T Ghrib **h23** Jiuba WEN **h24** Wenliang WANG **h25** Peng ZHANG **h27** Jingfeng SHAO

Date & Time	Room No. 1	Room No. 4	Room No. 3	Room No. 2	Room No. 5
01 JUNE (TUE)	**PARALLEL SESSIONS - 2**				
08:00 - 10:00	**Session B(b)** **Chairs:** ***Profs. Baicheng LIU & Bo WU***	**Session C(b)** **Chairs:** ***Profs. S Denis & M Reich***	**Session D(b)** **Chairs:** ***Profs. B Rivolta & Yanlin HE***	**Session E(b)** **Chairs:** ***Profs. M NARAZAKI & Ning YU***	**Session G(b)** **Chairs:** ***Profs. M Rachik & Wenya LI***
	B32 Yao SHEN **B25** Xueshao QIU **B24** Wei YOU **B06** Weimin GAO **B17** Likun ZHANG	**B20** **Jer-Ren YANG** **C03** M Reich **C08** Dongmei ZHU **C02** K Babu **C07** D Landek **C05** Guoyong LIU	**D41** **Fuxing YIN** **D14** Yongcheng LIN **D09** Yanlin HE **D12** Xudong ZHOU **D40** Ganlin XIE **D23** Jixiang ZHANG	**E16** **M Narazaki** **E07** J Ahlstrom **E08** F Frerichs **E10** MV LI **E13** Guanjie YUAN	**G01** Jianglin HUANG **G03** Huajun ZHANG **G05** Liang CHEN **G20** R Shateri **G02** Ali Slimani **D35** Huagui HUANG
10:00 - 10:30	***Coffee Break***				
01 JUNE (TUE)	**PARALLEL SESSIONS - 3**				
10:30 - 12:00	**Session B(c)** **Chairs:** ***Profs. Zhaohui JIN & Ping ZHANG***	**Session C(c)** **Chairs:** ***Profs. Jer-Ren YANG & BL Ferguson***	**Session D(c)** **Chairs:** ***Profs.Liwen ZHANG & Jixiang ZHANG***	**Session E(c)** **Chairs:** ***Profs. Young-Kook LEE & T UEHARA***	**Session G(c)** **Chairs:** ***Profs. Hsin-Chih LIN & Wenliang WANG***
	B21 **Xuejun JIN** **B08** Rongda ZHAO **B15** Zhenhuan ZHENG **B19** Tuo CHEN	**E05** **S MacKenzie** **C11** **Xiaodong HU** **H04** Min FENG **C13** MK Torbati	**B02** **B Rivolta** **D08** Weiming ZENG **D37** Xiao ZHAO **D38** Minjie LAI	**E15** Liu-Ho CHIU **E11** V Shchukin **E12** T Uehara	**G10** Lin MA **G12** Dejun KONG **B05** Yaogen SHEN **G19** Yi-Shiun DING
12:00 - 13:00	***Lunch***				

Date & Time	Room No. 1	Room No. 4	Room No. 3	Room No. 2	Room No. 5
01 JUNE (TUE)	**PARALLEL SESSIONS - 4**				
13:00 - 15:00	**Session B(d)** **Chairs:** ***Profs. Yao SHEN & Yaogen SHEN***	**Session C(d)** **Chairs:** ***Profs. Wei SHI & L Petrova***	**Session D(d)** **Chairs:** ***Profs. Dongyin JU & Huagui HUANG***	**Session F(a)** **Chairs:** ***Profs. P Gardin & Yitao YANG***	**Session F(b)** **Chairs:** ***Profs. NK Prabhu & Fuxing YIN***
	B31 **Jihua ZHANG** **B23** Maohua LIN **B14** Yongqiang LONG **B22** Chaohui ZHANG **B18** Guoxin YE	**C06** **Wei SHI** **C16** L Petrova **H09** Tei-Chen CHEN **C18** Jian XU **C20** N Svetushkov	**D16** **Liwen ZHANG** **D25** Yanshu ZHANG **D26** Yuewen ZHAI **D06** Jisen QIAO **D22** Lu LU **D05** Tingfang ZHANG	**F09** Shuang-Shii LIAN **F13** Xiaohua ZHAO **B01** P Gardin **F04** Shikun XIE **F12** Liang HE	**B04** Jianzheng GUO **F02** Lijia HE **F01** NK Prabhu **F06** Rongzhen XIAO **F05** Li WANG
15:00 - 15:30	***Coffee Break***				
01 JUNE (TUE)	**PARALLEL SESSIONS - 5**				
15:30 - 17:30	**Session H(a)** **Chairs:** ***Profs. Tei-Chen CHEN & I Potrc***	**Session H(b)** **Chairs:** ***Profs. Duc Hai Do & Sheng WANG***	**Session D(e)** **Chairs:** ***Profs. Lin CHEN & Z Pater***	**Session H(c)** **Chairs:** ***Profs. J Ahlstrom & Junxiao FENG***	**Session F(c)** **Chairs:** ***Profs. Shuang-Shii LIAN & Jianfeng GU***
	H07 Yu ZHANG **H10** Mei ZHANG **H11** Ying BA **H12** Yeqiong WU **H13** Guofei LIU **H20** Lei LU	**H01** B Samec **H02** G Oder **H03** Duc-Hai DO **H05** Haiwei ZHENG **H06** Zhiyin XIE **H19** Zhong ZHENG	**D13** Zhu SU **D18** Lin CHEN **D19** Lin CHEN **D20** Kun CHEN **D21** Dong HE **D36** Hua WANG	**H14** Guohua LI **H28** Zhibin SUN **H29** Sheng WANG **H15** Wenjun ZHAO **H16** Linghang XING **H18** Yanzhe LI	**F14** Enyu GUO **F08** Guiyong WU **F03** Baiyang LOU **F07** Hongmin GUO
18:00 - 20:00	***Conference Banquet***				

OPENING CEREMONY & PLENARY SESSIONS

31 May 2010 (Monday) Ballroom

Opening Ceremony 8:00 – 8:40

Chair: Prof. Weimin ZHANG
Prof. Wenjun ZHANG (SJTU President)
Dr. George E Totten (Conference Chair)
Dr. Robert B Wood (IFHTSE Secretary-General)

Session A(a) 08:40 – 09:50

Chair: Prof. Evan MA

08:40 – 09:15 **A1 George E Totten** (*Texas A&M University, USA*)
Process modeling for heat treatment: Current status and future developments

09:15 – 09:50 **A2 T Inoue** (*Fukuyama University*, *Japan*)
A mechanism of transformation plasticity and the identification of the characteristics

09:50 - 10:20 Coffee break

Session A(b) 10:20 – 12:05

Chair: Prof. T Inoue

10:20 – 10:55 **A4 Jianguo LIN** (*Imperial College London*, *UK*)
Hybrid forming processes for the production of lightweight high-strength automotive panel parts

10:55 – 11:30 **A7 Jian LU** (*The Hong Kong Polytechnic University, HK*)
Integrated design of product and component realized by thermal processes with pre-stressed engineering aproach

11:30 – 12:05 **A5 S Denis** (*LSG2M-UMR CNRS/INPL/UHP, France*)
Prediction of heat treatment residual stresses and distortions: Recent developments

12:05 - 13:00 Lunch

Session A(c) 13:00 – 14:45

Chair: Prof. Jian LU

13:00 – 13:35 **A6 Baicheng LIU** (*Tsinghua University, China*)
Modeling and simulation on deformation of heavy hydro turbine casting and heat trearment processes

13:35 – 14:10 **A3 Jiansheng PAN** (*Shanghai Jiao Tong University, China*)
Green heat treatment – the sustainable way of industrial developments

14:10 – 14:45 **A8 Evan MA** (*Johns Hopkins University, USA*)
Modeling amorphous structures produced by melt quenching: Zr-Cu-Al bulk metallic glass versus Ge-Sb-Te chalconenide phase-change glass

14:45 - 15:15 Coffee break

PARALLEL SESSIONS - 1

31 May 2010 (Monday) 15:15 – 17:00

Session B(a) Meeting room No. 1

Chairs: Profs. Xuejun JIN & Huiping LI

15:15 – 15:40 **B13 - Keynote Bo WU** (*Fuzhou University, China*)
A general approach on the order-disorder transition of complex intermetallics by combining thermodynamic model with first-principles calculations

15:40 – 16:00 **B12 Chaoyang SUN** (*University of Science and Technology Beijing, China*)
Experimental study of bainite transformation plasticity during continuous cooling for Armour steel

16:00 – 16:20 **B03 Zhuo YU** (*Leibniz University Hannover, Germany*)
Computation of the Isothermal Transformation Diagrams of 42CrMo4 Steel from the Dilatometer Measurements with Continuous Cooling

16:20– 16:40 **B10 Gangbo TANG** (*Central Iron and Steel Research Institute, China*)
Calculation on the incubation period of proeutectoid ferrite transformation for Si-Mn trip steel

16:40 – 17:00 **D11 Jun DING** (*Shanghai Jiao Tong University, China*)
String-like atomic motion in metallic glass under deformation

Session C(a) Meeting room No. 4

Chairs: Profs. S MacKenzie & D Landek

15:15 – 15:40 **E04 - Keynote BL Ferguson** (*Deformation Control Technology, Inc., USA*)
Using simulation for heat treat process design: Matching the quenching process with steel grade and product geometry

15:40 – 16:00 **C09 Zhichao LI** (*Deformation Control Technology, Inc.,USA*)
Computer modeling and validations of steel gear heat treatment processes using commercial software DANTE®

16:00 – 16:20 **C10 K Cvetkovski** (*Chalmers University of Technology, Sweden*)
Short-time tempering kinetics of quench hardened pearlitic steels

16:20 – 16:40 **C01 Weimin GAO** (*Deakin University, Australia*)
Integrated fluid-thermal-structure numerical analysis for the quenching of metallic components

16:40 – 17:00 **C14 Tao CONG** (*Harbin Institute of Technology, China*)
First principles characterization of phaseTi_2AlN prepared by plasma nitriding of Ti_3 Al alloy

Session D(a) Meeting room No. 3

Chairs: Profs. Jianguo LIN & A Gontarz

15:15 – 15:35 **D01 A Gontarz** (*Lublin University of Technology*, *Poland*)
Numerical analysis of unconventional forging process of hollowed shaft from Ti-6Al-4V alloy

15:35 – 15:55 **D02 Z Pater** (*Lublin University of Technology*, *Poland*)
The analysis of the cross-wedge rolling process of toothed shafts made from 2618 aluminium alloy

15:55 – 16:15 **D03 Haibo XIE** (*University of Wollongong*, *Australia*)
FEM temperature simulation of accelerated cooling on Run-out Table during hot rolling

16:15 – 16:35 **D04 Xiawei YANG** (*Harbin Institute of Technology*, *China*)
Fractal studies on primary phase morphology of the TA15 titanium alloy after hot compressive deformation

16:35 – 16:55 **D07 Jixiang ZHANG** (*Chongqing Jiaotong University, China*)
Research of Al-Mg-Si alloy hot-rolled multi-stage recrystallization by experiment and simulation

Session E(a) Meeting room No. 2

Chairs: Profs. Liu-Ho CHIU & T Luebben

15:15 – 15:40 **E01 - Keynote Young-Kook LEE** (*Yonsei University, Korea*)
Computer simulation of microstructure and distortion during quenching and tempering process of medium carbon steel

15:40 – 16:00 **E06 S MacKenzie** (*Houghton International, Inc., USA*)
Effect of alloy on the distortion of oil quenched automotive pinion gears

16:00 – 16:20 **E09 Dae-Hoon KO** (*Pusan National University, Korea*)
Prediction and measurement of residual stress for 6061 aluminum alloy during T6 heat treatment

16:20 – 16:40 **E02 T Luebben** (*Foundation Institute of Materials Science (IWT), Germany*)
Dimensional analysis of distortion during through hardening of cylindrical steel workpieces

16:40 – 17:00 **E03 J Rath** (*Foundation Institute of Materials Science (IWT), Germany*)
Generation of compressive residual stresses by high-speed water quenching

Session G(a) Meeting room No. 5

Chairs: Profs. Hao LU & Bolin HE

15:15 – 15:40 **G13 - Keynote Hsin-Chih LIN** (*National Taiwan University, Taiwan*)
The Surface Coatings of Super-Light Magnesium-Lithium Alloys

15:40 – 16:00 **G06 Yongcheng LIN** (*Central South University, China*)
Finite element model for the bonding process of anisotropic conductive films joints

16:00 – 16:20 **G07 Jihong YANG** (*Swinburne University of Technology, Australia*)
3D transient thermal modelling of the temperature profile during laser assisted machining of Ti6Al4V alloy

16:20 – 16:40 **G11 Changwen CUI** (*Fuzhou University, China*)
Three-dimensional numerical simulation of splat formation on substrates with different conditions in plasma spraying

16:40 – 17:00 **G09 Zhenhai XU** (*Harbin Institute of Technology, China*)
Deposition conditions effect on TiN film growth by molecular dynamics simulations

17:00 – 18:00 Supper

PARALLEL SESSIONS - 2

01 June 2010 (Tuesday) 08:00 – 10:00

Session B(b) Meeting room No. 1

Chairs: Profs. Baicheng LIU & Bo WU

08:00 – 08:20 **B32 Yao SHEN** (*Shanghai Jiao Tong University, China*)
The effects of coherency stress on interdiffusion across coherent multilayer interfaces

08:20 – 08:40 **B25 Xueshao QIU** (*Zhengzhou University of Light Industry, China*)
The reconstruction of the temperature field base on Matlab and two-dimensional interpolation

08:40 – 09:00 **B24 Wei YOU** (*North China Institute of Science and Technology, China*)
Predicting the CCT Diagrams of Steels Using Artificial Neural Network Models

09:00 – 09:20 **B06 Weimin GAO** (*Deakin University, Australia*)
Modelling hydrogen diffusion and phase transformation for titanium powder hydrogenization-dehydrogenization (HDH) rolling process

09:20 – 09:40 **B17 Likun ZHANG** (*Fuzhou University, China*)
Prediction of the site occupancy of alloying elements in REFe12-xMx-based alloy with ThMn12 prototype by combining thermodynamic model with first-principles calculations

Session C(b) Meeting room No. 4

Chairs: Profs. S Denis & M Reich

08:00 – 08:25 **B20 - Keynote Jer-Ren YANG** (*National Taiwan University*)
The heat treatment of superbaintic ferrite

08:25 – 08:45 **C03 M Reich** (*University of Rostock*, *Germany*)
Mechanical properties of undercooled aluminium alloys and their implementation in quenching simulation

08:45 – 09:05 **C08 Dongmei ZHU** (*University of Science and Technology Beijing, China*)
Numerical simulation research on heat transfer of air mist spray cooling

09:05 – 09:25 **C02 K Babu** (*Indian Institute of Technology Madras, India*)
Finite element modeling of quenching heat treatment of AISI 4140 steel with phase transformation

09:25 – 09::45 **C07 D Landek** (*University of Zagreb, Croatia*)
Prediction of properties of gas-quenched work pieces based on the modified hardenability test

09::45 – 10:05 **C05 Guoyong LIU** (*University of Science and Technology Beijing, China*)
Influencing factors on cooling uniformity of large caliber seamless pipe for quenching

Session D(b) Meeting room No. 3

Chairs: Profs. B Rivolta & Yanlin HE

08:00 – 08:25 **D41- Keynote Fuxing YIN** (*National Institute for Materials Science, Japan*)
Hot-rolling bonded multilayered composite steels and the varied tensile deformation behavior

08:25 – 08:45 **D14 Yongcheng LIN** (*Central South University, China*)
Numerical simulation for effects of friction on quality of low alloy steel forgings

08:45 – 09:05 **D09 Yanlin HE** (*Shanghai University, China*)
Influence of soaking temperature on microstructure of multi-pass compression deformation for low carbon steels

09:05 – 09:25 **D12 Xudong ZHOU** (*Henan University of Science and Technology, China*)
The forging penetration efficiency of steel H13 stepped shaft radial forging with GFM forging machine

09:25 – 09:45 **D40 Ganlin XIE** (*University of Science and Technology Beijing, China*)
Microstructural modeling of dynamic recrystallization in Nb microalloyed steels

09:45 – 10:05 **D23 Jixiang ZHANG** (*Chongqing Jiaotong University, China*)
A novel Monte Carlo Potts Model in metal recrystallization simulation

Session E(b) Meeting room No. 2

Chairs: Profs. M Narazaki & Ning YU

08:00 – 08:25 **E16 - Keynote M Narazaki** (*Utsunomiya University, Japan*)
Simulation of asymmetrical quench distortion of long thin steel parts

08:25 – 08:45 **E07 J Ahlström** (*Chalmers University of Technology, Sweden*)
Modelling of distortion during cooling and machining of aluminium engine blocks with cast-in cast iron liners

08:45 – 09:05 **E08 F Frerichs** (*Stiftung Institut für Werkstofftechnik, Germany*)
Effects of Inhomogeneous Distributions of Distortion Potential on Out of Roundness of Rings

09:05 – 09:25 **E10 MV LI** (*Portland State University, USA*)
Microstructure evolution and residual stresses in coke drum repair welds

09:25 – 09:45 **E13 Guanjie YUAN** (*University of Science and Technology Beijing, China*)
Finite element modeling of hydrostatic stresses distribution in copper dual-damascene interconnects

Session G(b) Meeting room No. 5

Chairs: Profs. M Rachik & Wenya LI

08:00 – 08:20 **G01 Jianglin HUANG** (*University of Birmingham, UK*)
Modelling of hydrogen effect on porosity formation in electron beam welded titanium-based alloys

08:20 – 08:40 **G03 Huajun ZHANG** (*Harbin University of Science and Technology*, *China*)
Stress and distortion of simultaneous control by two-sided arc welding for thick plate of high strength steel

08:40 – 09:00 **G05 Liang CHEN** (*Northwestern Polytechnical University*, *China*)
Effects of processing parameters on the temperature field and axial shortening of inertia friction welded GH4169 joints by numerical simulation

09:00 – 09:20 **G20 R Shateri** (*Islamic Azad university, Iran*)
Effect of solution annealing in post and preheat conditions on microstructure and mechanical properties of IN-718 weld metal

09:20 – 09:40 **G02 Ali Slimani** (*Compiegne University of Technology, France*)
High temperature indentation test to improve constitutive model for welding simulation

09:40 – 10:00 **D35 Huagui HUANG** (*Yanshan University, China*)
Research on pores deformation welding condition for manufacturing of heavy forings

10:00 – 10:30 Coffee Break

PARALLEL SESSIONS - 3

01 June 2010 (Tuesday) 10:00 – 12:00

Session B(c) Meeting room No. 1

Chairs: Profs. Zhaohui JIN & Ping ZHANG

10:30 – 10:55 **B21- Keynote Xuejun JIN** (*Shanghai Jiao Tong University*, *China*)
Microstructure design and implementation of new generation high strength multi-phase steels

10:55 – 11:15 **B08 Rongda ZHAO** (*Harbin Institute of Technology Harbin, China*)
The formation of nanometer coherent structures during spinodal decomposition and ordering coexistence phase transformation in Fe-24Al alloys

11:15 – 11:35 **B15 Zhenhuan ZHENG** (*Fuzhou University, China*)
Prediction of the site occupancies of alloying elements in D019-type Ti3Al-based alloy by combining thermodynamic model with ab initio Calculations

11:35 – 11:55 **B19 Tuo CHEN** (*Fuzhou University, China*)
Prediction of the ordering behaviors of alloying elements Ta, V, Mo and Hf in Ti2AlNb-based orthorhombic alloy by combining thermodynamic model with ab initio calculations

Session C(c) Meeting room No. 4

Chairs: Profs. Jer-Ren YANG & BL Ferguson

10:30 – 10:55 **E05 - Keynote S MacKenzie** (*Houghton International, Inc.*, *USA*)
Comparison between High Pressure Hydrogen Quenching and Oil Quenching of Steel Parts Considering Load Effect (***Present in "C"***)

10:55 – 11:20 **C11- Keynote Xiaodong HU** (*Saitama Institute of Technology, Japan*)
The Developments and application of computer simulation code on Induction heat treatment process

11:20 – 11:40 **H04 Min FENG** (*Dalian Maritime University, China*)
Phase diagram simulation and heat-treatment of a Ni-based alloy for high-temperature vitriol pump

11:40 – 12:00 **C13 MK Torbati** (*Ferdowsi University of Mashhad, Iran*)
Thermodynamic analytical modeling of gas reactions to investigate the effect of environmental temperature and humidity on carbon potential in gas carburizing process

Session D(c) Meeting room No. 3

Chairs: Profs. Liwen ZHANG & Jixiang ZHANG

10:30 – 10:55 **B02 - Keynote B Rivolta** (*Politecnico di Milano*, *Italy*)
Recrystallization kinetics of austenite in Nb microalloyed steel

10:55 – 11:15 **D08 Weiming ZENG** (*Shanghai University, China*)

Recrystallization behavior of a Ti-microalloyed complex phase steel during hot compression

11:15 – 11:35 **D37 Xiao ZHAO** (*Northwestern Polytechnical University, China*)
Numerical analysis of the effect of material properties on the deformability of near hemispherical shell

11:35 – 11:55 **D38 Minjie LAI** (*Northwestern Polytechnical University, China*)
First-principles prediction of ductility in β-type Ti-Mo binary alloys

Session E(c) Meeting room No. 2

Chairs: Profs. Young-Kook LEE & T Uehara

10:30 – 10:50 **E15 Liu-Ho CHIU** (*Tatung University, Tanwan*)
Distortion measurement of martensitic stainless mold steels by vacuum heat treatment

10:50 – 11:10 **E11 V Shchukin** (*Khristianovich Institute of Theoretical and Applied Mechanics, Russia*)
Numerical modeling of the stress-and-strain state of the surface layer of steel at high-frequency pulse treating

11:10 – 11:30 **E12 T Uehara** (*Yamagata University, Japan*)
Computer simulation of microscopic stress distribution in complex microstructure using a phase field model

Session G(c) Meeting room No. 5

Chairs: Profs. Hsin-Chih LIN & Wenliang WANG

10:30 – 10:50 **G10 Lin MA** (*Academy of Armored Force Engineering, China*)
The analysis of stress and strain field of the laser cladding process on the ring circular orbit

10:50 – 11:10 **G12 Dejun KONG** (*Jiangsu Polytechnic University, China*)
Structures and properties of VC coating on Cr12MoV cold working die surface steel by TD process

11:10 – 11:30 **B05 Yaogen SHEN** (*City University of Hong Kong*, *HK*)
Size-dependent lognormal grain size distribution in nanocomposite films

11:30 – 11:50 **G19 Yi-Shiun DING** (*National Taiwan Ocean University, Taiwan*)
Notched tensile fracture of Ti-15V-3Cr-3Sn-3Al Alloy welds

12:00 - 13:00 Lunch

PARALLEL SESSIONS - 4

01 June 2010 (Tuesday) 13:00 – 15:00

Session B(d) Meeting room No. 1

Chairs: Profs. Yao SHEN & Yaogen SHEN

13:00 – 13:25 **B31 - Keynote Jihua ZHANG** (*Shanghai Jiao Tong University, China*)
Microstructural evolution of two way hysteresis-free shape memory effect in Mn-based antiferromagnetic alloys

13:25 – 13:45 **B23 Maohua LIN** (*Fuzhou University*, *China*)
Design of magnetic high entropy alloy with FCC structure by combining thermodynamic model with first-principles calculations

13:45 – 14:05 **B14 Yongqiang LONG** (*Henan University of Science and Technology, China*)
First-principles investigation of the structural stability and electronic property of precipitates on the Cu-rich side of Cu-Ni-Si alloys

14:05 – 14:25 **B22 Chaohui ZHANG** (*Fuzhou University, China*)
Design of high entropy alloy with FCC structure by combining thermodynamic model with first-principles calculations

14:25 – 14:45 **B18 Guoxin YE** (*Fuzhou University, China*)
Prediction of the site occupancy of alloying elements in Ni3Al-based L12 alloy by combining thermodynamic model with first-principles Calculations

Session C(d) Meeting room No. 4

Chairs: Profs. Wei SHI & L Petrova

13:00 – 13:25 **C06 - Keynote Wei SHI** (*Tsinghua University*, *China*)
Modeling of transformation plasticity during quenching processes of large steel forgings and experimental validation

13:25 – 13:45 **C16 L Petrova** (*Moscow State Automobile and Road Construction State Technical University, Russia Federation*)
Modeling of processes of thermo-chemical treatment: Traditions of Russian Scientific School

13:45 – 14:05 **H09 Tei-Chen CHEN** (*National Cheng Kung University, Taiwan*)
Nanoscale mechanical behaviors of nanostructured silicon

14:05 – 14:25 **C18 Jian XU** *(University of Science and Technology Beijing, China)*
Numerical simulation for thermal process upon reducing gas composition of pre-reduction shaft furnace

14:25 – 14:45 **C20 N Svetushkov** (*Moscow State Automobile and Road Institute, Russia*)
Geometric integral methods in simulation of thermal processes

Session D(d) Meeting room No. 3

Chairs: Profs. Dongying JU & Huagui HUANG

13:00 – 13:25 **D16 - Keynote Liwen ZHANG** (*Dalian University of Technology, China*)
3D Finite Element Simulation of Rod and Wire Continuous Rolling

13:25 – 13:45 **D25 Yanshu ZHANG** (*Advanced Manufacture Technology Center, China Academy of Machinery Science& Technology, China*)
The Microstructure prediction of magnesium alloy AZ31D during hot extrusion

13:45 – 14:05 **D26 Yuewen ZHAI** (*Beijing Research Institute of Mechanical & Electrical Technology, China*)
The application of numerical simulation technology to the forming process of large scale tee

14:05 – 14:25 **D06 Jisen QIAO** (*State Key Laboratory of Gansu Advanced Non-ferrous Metal Materials, China*)
Study on temperature evolution and metal flow of 6005A aluminum alloy during indirect hot extrusion

14:25 – 14:45 **D22 Lu LU** (*Tianjin Polytechnic University, China*)
Simulation of the tube forming process in Mannesmann mill

14:45 – 15:05 **D05 Tingfang ZHANG** (*Nanchang University*, *China*)
Simulation experiment on friction coefficients during warm deep drawing of magnesium alloy sheet

Session F(a) Meeting room No. 2

Chairs: Profs. P Gardin & Yitao YANG

13:00 – 13:20 **F09 Shuang-Shii LIAN** (*National Taiwan University* ,*Taiwan*)
Simulation study of the effects of parameters of graphite susceptor for induction metling process of polycrystalline silicon

13:20 – 13:40 **F13 Xiaohua ZHAO** (*Northwestern Polytechnical University, China*)
Numerical simulation of fluid flow caused by buoyancy forces during VAR process

13:40 – 14:00 **B01 P Gardin** (*Arcelor Mittal Global R&D*, *France*)
Mathematical modeling: an efficient way to predict inclusion evolution in liquid steel

14:00 – 14:20 **F04 Shikun XIE** (*Jinggangshan University, China*)
Remelting technology and microstructural evolution of semi-solid Al-7Si-2RE alloy

14:20 – 14:40 **F12 Liang HE** (*Worcester Polytechnic Institute, USA*)
Modeling on Directional Solidification of Solar Cell Grade Multicrystalline Silicon Ingot Casting

Session F(b) Meeting room No. 5

Chairs: Profs. NK Prabhu & Fuxing YIN

13:00 – 13:20 **B04 Jianzheng GUO** (*ESI US R&D, USA*)
Prediction of microstructure and mechanical properties in aluminum castings after heat treatment

13:20 – 13:40 **F02 Lijia HE** (*Liaoning University of Technology, China*)
Modification analysis of hypereutectic Al-Si alloy with P or phosphide by EET

13:40 – 14:00 **F01 NK Prabhu** (*National Institute of Technology Karnataka, India*)
Measurement of heat transfer coefficients during downward solidification of commercially pure Zn and ZA8 alloy

14:00 – 14:20 **F06 Rongzhen XIAO** (*Lanzhou University of Technology, China*)
Phase-field modeling of free dendritic growth in a binary alloy under a forced flow

14:20 – 14:40 **F05 Li WANG** (*Tsinghua University, China*)
Numerical simulation of macrosegregation during steel ingot solidification using continuum model

15:00 – 15:30 Coffee break

PARALLEL SESSIONS - 5

01 June 2010 (Tuesday) 15:30 – 17:30

Session H(a) Meeting room No. 1

Chairs: Profs. Tei-Chen CHEN & I Petrc

15:30 – 15:50 **H07 Yu ZHANG** (*University of Science and Technology Beijing, China*)
Development and application of thermal mathematical model of iron ore pellet bed in grate

15:50 – 16:10 **H10 Mei ZHANG** (*Shanghai University, China*)
High temperature mechanical properties of a Ti-microalloyed complex phase steel

16:10 – 16:30 **H11 Ying BA** (*Harbin Institute of Technology, China*)
Thermo-elasto-plastic damage analysis of functionally graded materials under thermal loading

16:30 – 16:50 **H12 Yeqiong WU** (*Harbin Institute of Technology, China*)
Properties and electronic structure of iron under pressure up to 30GPa

16:50 – 17:10 **H13 Guofei LIU** (*University of Mining and Technology (Beijing), China*)
Numerical simulation of defect inspection using electromagnetic stimulated thermography

17:10 – 17:30

17:30 – 17:50 **H20 Lei LU** (*Inner Mongolia University of Technology, China*)
A symmetry-homotopy hybrid algorithm for solving boundary value problem of partial differential equations

Session H(b) Meeting room No. 4

Chairs: Profs. Duc Hai Do & Sheng WANG

15:30 – 15:50 **H01 B ŠAMEC** *(University of Maribor, Slovenia)*
Numerical analysis of a railway brake disc

15:50 – 16:10 **H02 Grega Oder** *(University of Maribor, Slovenia)*
Numerical analysis of braking discs for a »Taurus« class locomotive

16:10 – 16:30 **H03 Duc Hai Do** (*Magdeburg University, Germany*)
Mathematical modelling and simulation of lime burning process in a normal shaft kiln

16:30 – 16:50 **H05 Haiwei ZHENG** (*University of Science and Technology Beijing, China*)
Optimization of pellet production process parameters in grate using simulation results

16:50 – 17:10 **H06 Zhiyin XIE** (*University of Science and Technology Beijing*, *China*)
Optimization of pellet induration process parameters in rotary kiln using simulation results

17:10 -17:30 **H19 Zhong ZHENG** (*Hubei University of Technology, China*)
Effects of conformal cooling channel on injection molding and productivity

Session D(e) Meeting room No. 3

Chairs: Profs. Lin CHEN & Z Pater

15:30 – 15:50 **D13 Zhu SU** (*Chongqing University, China*)
Thermal-mechanical coupling simulation and springback control in hot forming process of fan blade

15:50 – 16:10 **D18 Lin CHEN** (*Inner Mongolia university of science and technology, China*)
Numerical simulation analysis in cooling temperature field and bending deformation after rolling of 100-meter rail

16:10 – 16:30 **D19 Lin CHEN** (*Inner Mongolia university of science and technology, China*)
Research and Application of Pre-bent automatic control Models of 100 meters rail

16:30 – 16:50 **D20 Kun CHEN** (*Shanghai University, China*)
Simulation of large forging flat-anvils stretching process and its optimization

16:50 – 17:10 **D21 Dong HE** (*Harbin Institute of Technology, China*)
A study of FCC metal tension behavior by crystal plasticity finite element method

17:10 – 17:30 **D36 Hua WANG** (*Shanghai University, China*)
FEM study of the tensile behavior of annealed ULC-BH steels

Session H(c) Meeting room No. 2

Chairs: Profs. J Ahlstrom & Junxiao FENG

15:30 – 15:50 **H14 Guohua LI** (*China University of Mining & Technology（Beijing）, China*)
Numerical Simulation of the NDT of Metallic Composites Plate by Infrared Thermography

15:50 – 16:10 **H28 Zhibin SUN** (*University of Science and Technology Beijing, China*)
Optimization of pellet production process parameters in annular cooler using simulation results

16:10 – 16:30 **H29 Sheng WANG** (*RIKEN, Japan*)
Performance, flow and thermal characteristics of a viscous micro/nano pump simulated by particle/continuum methods

16:30 – 16:50 **H15 Wenjun ZHAO** (*Harbin Institute of Technology, China*)
Modeling of recirculation zone around the nozzle used in spray forming

16:50 – 17:10 **H16 Linghang XING** (*Changjiang Sciendific Research Institute, China*)
Modified QUICK schemes for 3D advection-diffusion equation of pollutants on unstructured grids

17:30 – 17:50 **H18 Yanzhe LI** (*Lanzhou Jiao Tong University, China*)
Modeling and simulation for electromagnetic shielding performance of magnesium

Session F(c) Meeting room No. 5

Chairs: Profs. Shuang-Shii LIAN & Jianfeng GU

15:30 – 15:50 **F14 Enyu GUO** (*Tsinghua University, China*)
Modeling and simulation of solidification and temperature of thick-wall stainless steel pipe in horizontal centrifugal casting process

15:50 – 16:10 **F08 Guiyong WU** (*Dalian University of Technology, China*)
Numerical simulation of structure and shrinkage in cast-steel ingot

16:10 – 16:30 **F03 Baiyang LOU** (*Zhejiang University of Technology, China*)
Numerical simulation of mold filling and solidification process of a disc aluminum alloy in pressure die casting

16:30 – 16:50

16:50 – 17:10 **F07 Hongmin GUO** (*Nanchang University, China*)
Micro-scale modeling of soft impingement during rheocasting

18:00 – 20:00 Conference banquet

POSTER SESSIONS

01 June 2010 (Tuesday) 18:30 – 21:30 Meeting room No. 1

B SESSION – Phase transformation & Alloy design

b09 **Jing WU** (*Shanghai University, China*)
Study on the initiation and evolution of strengthening phase in niobium micro-alloyed steel by 3DAP

b11 **Naqiong ZHU** (*Shanghai University, China*)
Modeling of nucleation and growth of $M_{23}C_6$ carbidein multi-component Fe-based alloy

b16 **Xiangying MENG** (*Northeastern University, China*)
First-principles calculation of the temperature dependence of hardening precipitation in Mg-Gd alloys

b26 **Shikun XIE** (*Jinggangshan University, China*)
Process of Equiaxed Grains of RE-Al Alloy under Slope Vibration

b27 **Shanglei YANG** (Shanghai University of Engineering Science*, China*)
Calculation on the solid solution forming enthalpies of Re-Mo-Ti gradient alloy in thermodynamics

b28 **Hong DING** (*Shanghahi Jiao Tong University, China*)
Monte Carlo study of B2-$L2_1$ ordering transitions in Au-Cu-Al systems

b30 **Ping DONG** (*National Key Laboratory Surface Physics and Chemistry, China*)
Numerical simulation of temperature and stress fields in beryllium cutting process

b33 **Ning YU** (*Shanghai Jiao Tong University, China*)
Simulating mechanical behaviour of porous materials for SOFC

C SESSION – Heat treatment

c15 **H Yahagi** (*Saitama Institute of Technology, Japan*)
Thermal flow simulation and visualization of PAG quenchants in cooling evaluation equipment with twin stir

c19 **Huiping LI** (*Shandong University, China*)
Research on the quenching performance of 22MnB5 quenched in the steel die

c21 **Xunwei ZUO** (*Shanghai Jiao Tong University, China*)
Timed quenching process for large-scale AISI4140 steel shaft

c22 **Yingli ZHAO** (*Kunming University of Science and Technology, China*)
Kinetics of austenite grain growth in medium-carbon Nb-bearing steel

c23 **Dongying JU** (*Saitama Institute of Technology, Japan*)
The developments and application of computer simulation code on induction heat treatment process

c24 **Ruikai CHEN** (*Shanghai Jiao Tong University, China*)
A noval process to refine the grain size of NiCrMoV steel

D SESSION – Deformation & Recrystallization

d10 Xiangru LIU (*Henan University of Science & Technology，China*)
The study of warm surface rolling of steel 45 groove axle

d15 Ben ZENG (*Shanghai University, China*)
Simulation on rolling force and temperature field of plate steel during hot rolling

d17 Lin CHEN (*Inner Mongolia university of science and technology, China*)
Dynamic recrystallization model and simulation analysis of SPCC steel hot rolling

d27 Guanyu DENG (*University of Wollongong, Australia*)
Orientation evolution during equal channel angular pressing of aluminum single crystal

d29 Shu GUO (*Harbin Institute of Technology, China*)
Simulation of hot deformation of spray formed 7XXX alloy with high Zn content

d30 Junqing GUO (*Henan University of Science and Technology, China*)
Study on Computer Simulation and Superplastic Extrusion of AZ31B Seamless Tube

d31 Xiaochun MA (*Zhejiang University of Technology, Hangzhou, China*)
Study on the finite element numerical simulation of automobile beam stamping forming

d32 Junguang HE (*Henan University of Science and Technology, China*)
Computer simulations of the continuous annealing recrystallization for cold rolled strip steel in galvanizing line

d33 Lei ZHANG (*Shandong University, China*)
Numerical simulation of U-channel forming process of quenchable steel at elevated temperature

d34 Yu ZHANG (*Chongqing Jiaotong University, China*)
Design of flash structure for forging die based on intelligent optimization algorithms

d39 Bin TANG (*Northwestern Polytechnical University, China*)
Asymmetric deformation of near hemispherical diaphragm under uniform surface load: Simulation and Experimental

d42 Yongge FAN (*Southwest University of Science and Technology, China*)
Numerical simulation of expanding process for hollow billet during extrusion steel tube

F SESSION – Melting & Casting

f11 Yitao YANG (*Shanghai University, China*)
The establishment of some particular methods in casting simulation

f15 Zhijun YANG (*Northwestern Polytechnical University, China*)
Numerical simulation of temperature distribution and heat transfer during the solidification of Ti-6Al-4V ingots in VAR process

G SESSION – Welding & Coating

g04 **Yansong ZHANG** (*Shanghai Jiao Tong University, China*)
The effect of post heating on Nugget quality for spot welding dual phase steels using FE and experimental methods

g08 **A Sliwa** (*Silesian University of Technology, Poland*)
Finite element method application for modeling of PVD coatings Properties

g14 **Yong SUN** (*University of Wollongong, Australia*)
Molecular dynamics simulation of bonding at the Fe-Al interface

g15 **Bolin HE** (*East China Jiaotong University, China*)
Effects of crack opening angle and external loads on the reliability of welded pipe with circumferential crack

g16 **Wen-Ya LI** (*Northwestern Polytechnical University, China*)
Modeling of the whole friction stir welding process by the explicit finite element method

g17 **Yong HU** (*East China Jiaotong University, China*)
Numerical simulation of semisolid die casting process of magnesium alloy

g18 **Zhi ZHANG** (*Naval University of Engineering, Wuhan, China*)
Analysis of Temperature－Stress Coupling Field in Laser Cladding Process with Powder Feeding

H SESSION – Miscellaneous

h08 **Yinghua JIANG** (*Dongbu Steel Co. Ltd, Korea*)
Evaluation model of susceptibility to hot shortness of Cu-containing LC steel

h21 **Yu-Sen YANG** (*National Kaohsiung First University of Science and Technology, Taiwan*)
A study of the measurement method of spheroidizing rate on coils of low carbon steel

h22 **T Ghrib** (*Photothermal Laboratory, IPEIN, Tunisia*)
Detection of Surface Defects by the Photothermal Deflection

h23 **Jiuba WEN** (*Henan University of Science and Technology, China*)
Analysis of Electrochemical Noise and Physical Model of Corrosion Process of Al-Zn-In Series Alloys in NaCl Solutions

h24 **Wenliang WANG** (*Nanchang University, China*)
Simulated annealing algorithm and optical thin film

h25 **Peng ZHANG** (*Harbin Institute of Technology at Weihai, China*)
FEM-based thermo-physical process of laser spot heating of sheet metal

h27 **Jingfeng SHAO** (*Xi'an Polytechnic University, China)*
Development and modeling of production management and decision analysis system for finishing workshop based on multi-agent

A01

Process Modeling For Heat Treatment: Current Status and Future Developments

G.E. Totten[1], J. Gu[2], J.S. Pan[2]
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2. Shanghai Jiaotong University, Department of Materials Science, Shanghai, China
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Modeling and computer simulation of material manufacturing processes is an interdisciplinary field gaining in ever-increasing attention worldwide. In fact, this is one of the most critical research areas in the field of material and processing technology. There have been continuous developments in modeling and simulation processes within the forging and casting industries over the past 40 years and, as a result, modeling of these processes is now widely used in industrial product and process design and production. Considerable progress was made in fundamental and theoretical research of modeling and simulation. Numerous mathematical models have been proposed and improved which has led to the introduction of commercial software which has greatly impacted productivity. However, existing models and software cannot meet the demands of the continuing development needs of modern manufacturing technological advances. An overview of potential barriers to the continued growth and applicability of thermal process modeling and simulation in support of industrial product and process design and application is provided here.

Keywords: *Modeling, Simulation*

A02

Mechanism of Transformation Plasticity and the Identification of the Characteristics

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A phenomenological mechanism of transformation plasticity (TP) [1-3] is discussed from the viewpoint of thermoplasticity, in the first part of the paper, why it takes place under a stress level even lower than the characteristic yield stress of mother phase. This is principally based on the difference in thermal expansion coefficient in new and mother phases. Bearing in mind that it is also a kind of plastic strain, a unified plastic flow theory is derived by introducing the effect of progressing new phase into the yield function of stress, temperature and plasticity related parameters, which gives the generalized Greenwood-Johnson formula for evolution of transformation plastic strain rate. Experimentally identified TP coefficient are presented in the following section for some steels under tensile and compressive stress.

As examples of the application of the theory and the data, metallo-thermo-mechanical simulations by use of developed code COSMAP [4] available for quenching process are also carried out for blank gear wheel, plastically bent thin plate and Japanese sword to demonstrate how the effect of TP is drastically influenced in the simulation.

Keywords: *transformation plasticity, unified transformation-thermoplasticity theory, metallo-thermo-mechanics, quenching*

References:

[1] Greenwood, G.W. and Johnson, R.H., The deformation of metals under small stresses during phase transformations, Proc. Roy. Soc., Vol. 283A, 1965, pp.403-422.
[2] Inoue, T., Unified transformation-thermoplasticity and the application, J. Soc. Materials Science, Japan, Vol.56, 2007, pp.354-358.
[3] Inoue, T., Mechanism of Transformation Plasticity and the Unified Constitutive Equation for Trans-formation-Thermo-Mechanical Plasticity with Some Applications, Proceedings of 2 nd International Conference on Distortion Engineering, Bremen (2008) pp.375-382
[4] Ju, D-Y., and Inoue, T., Simulation and its experimental verification by the Material Process CAE Code COSMAP,

Proceedings of 2 nd International Conference on Distortion Engineering, Bremen (2008) pp.441-450

A04

Hybrid forming processes for the production of lightweight high-strength automotive panel parts

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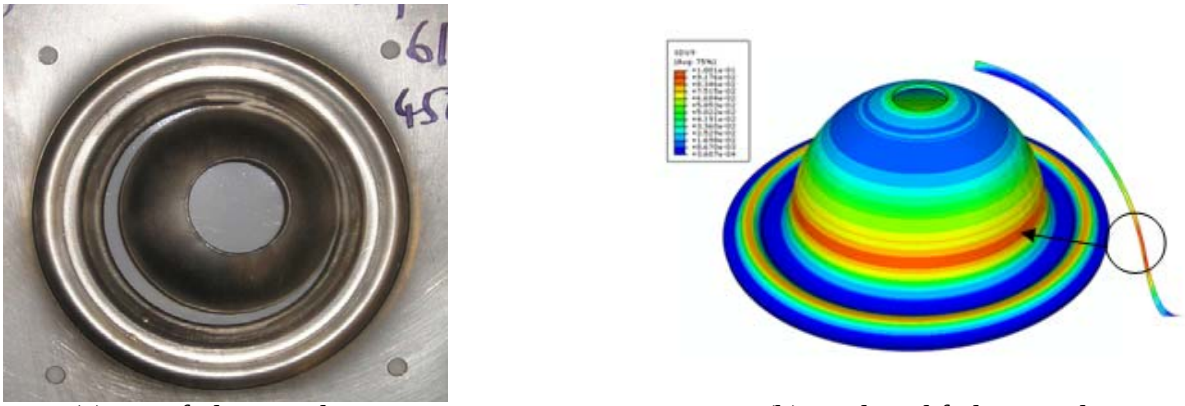
In the automotive industry, there is an ever increasing need to increase the safety by using stronger components and reduce CO_2 emission via weight reduction. Recently hot stamping and cold die quenching processes have been developed for the forming of lightweight high strength panel components particularly targeted for automotive applications. The research concentrates on two types of materials: one is the boron steel and the other is heat treatable and non-heat-treatable aluminium alloys. In terms of the steel, research results on the modelling of austenisation during heating and bainite and martensite transformation during cooling are reported. Regarding aluminium alloys, the modeling work will be concentrated on the precipitate formation and growth features. For both the steel and aluminium alloys, viscoplastic damage constitutive equations are also developed and determined from their experimental data for the prediction of viscoplastic flow and ductility of the materials. The determined unified constitutive equations are then implemented into the commercial Finite Element code Abaqus/Explicit via the user defined subroutine, VUMAT. An FE process simulation model and numerical procedures are established for the modelling of a hot stamping and cold die quenching processes for a spherical part with a central hole. Different failure modes (failure takes place either near the central hole or in the mid span of the part) are obtained. To validate the simulation results, a test programme is developed, a test rig has been designed and manufactured, and tests have been carried out for the materials with different forming rates. It has been found that very close agreements between experimental and numerical process simulation results are obtained for the range of temperature and forming rates carried out. The following figure shows an example for the comparison of experimental and simulation results for AA6082.



(a) Test failure mode (b) Predicted failure mode

Figure 1. Comparison of (a) Experimental and (b) predicted failure modes for the part formed at the forming rate of 170mm/s.

A06

Stress Analysis and Deformation Prediction of a Heavy Hydraulic Turbine Blade Casting During Casting and Heat Treatment

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The blade casting is one of main components for heavy hydro turbines. This casting, a kind of large and curved shape, is susceptible to deformation during casting and heat treatment processes. In this paper, the modeling and simulation is performed for the stress analysis of a blade casting during casting and heat treatment processes. The coupled thermo-phase transformation-stress and thermo-stress models are used for casting and heat treatment process, respectively. Machining allowance distribution is used as the deformation criterion and the algorithm of inverse deformation determination is presented. The mechanical properties of the material matensitic stainless steel ZG0Cr13Ni4Mo (Cr13%, Ni5%, Mo1%) at different temperatures and with as-cast and heat treated microstructures are measured. Finally, the inverse deformation of the blade during both casting and heat treatment processes is obtained. And the sections of the blade casting with inverse deformation design are given for the pattern making. The calculated deformations are compared to the measured results and they are basically in agreement.

Keywords: *Turbine blade, Casting, Heat treatment, Phase transformation, Stress, Deformation*

A07

Integrated design of product and component realized by thermal processes with pre-stressed engineering approach

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This work will summarized the development of a global approach to integrate the residual stresses induced by the thermal process for controlling and optimising important mechanical properties such as fatigue, wear and stress corrosion cracking. As applications, we can mention: heat treatment and thermochemical processing (quenching, carburizing, nitriding), welding, machining, laser forming thermal spray and composite etc. This approach explores the way to introduce prestress processing in the design of mechanical components and structures. In fact, the development of a global approach with associated CAD-CAM tools is necessary to ease the collaboration between the engineers working on material choice, production design and quality control.

Residual stress considerations are becoming important today for two reasons: the necessity for the designer to reduce the weight of the structure and keep the same safety level to be competitive and the introduction of multimaterials which induces residual stress. With the development of different numerical simulation tools and experimental techniques, it is now possible to consider residual stress issues in the design office for the integrated design of mechanical components. A new approach of concurrent engineering applied to the design of mechanical components with the residual and applied stresses consideration will be presented. Different examples in key industrial sectors such as energy, aircraft, automotive will be presented. In the aerospace industry, the mastering of residual stresses could lead to a decrease in the weight of aircraft structures and consequently reduce the consumption of fuel in the same proportions. In the automotive and mechanical industries, the mastering of different surface treatments on mechanical parts with high loads could improve performances characteristics and increase the lifetime of mechanical parts. The fatigue life

design time of mechanical components could be reduced about 50%. In the power generation industry, improvements in methodologies for taking residual stress into account could lead to a reduction in degradation or failures due to mechanical fatigue or due to environmentally assisted corrosion cracking because conventional design strategies do not consider the existence of residual stresses. The measurement and control of residual stresses, e.g. in welded parts of structural components, such as piping systems and pressure vessels, leads to a significant improvement of plant availability and increase of plant safety. Furthermore mastering residual stresses would lead to a reduction of the number of operation in the control procedure required for large structural parts and reduce the repair cost.

Finally, the future orientations of the pre stressed engineering will be presented.

Keywords: *Numerical simulation, prestressed engineering, fatigue, measurement techniques*

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A08

Modeling amorphous structures produced by melt quenching: Zr-Cu-Al bulk metallic glass versus Ge-Sb-Te chalcogenide phase-change glass

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Using molecular dynamics and ab initio molecular dynamics simulations, we compare the atomic-level structure in the Zr-Cu-Al (Y.Q. Cheng et al., PRL 2009), a typical bulk metallic glass former, with that in the amorphous Ge2Sb2Te5 (M. Xu et al., PRL 2009), a prototype phase-change alloy for data storage (e.g., in DVD). These glasses were obtained by quenching from the melt in the computer models. We found that the Zr-Cu based BMGs can be pictured as composed of densely packed (due to metallic bonding) Cu-centered icosahedra, w/ local motifs distinctly different from crystals. Al plays a special role, both in terms of chemistry and topology: the stabilizing effect of Al is not merely topological, but also has its origin in the electronic interactions and bond shortening. These structural features suggest slow dynamics and high barrier to cyrstallization, leading to a good (bulk) glass former. In contrast, the Ge2Sb2Te5 (GST) glass is semiconducting and characterized by p bonding. Electronic structure calculations reveal a global valence alternation. The resulting p bonding profoundly influences the local atomic structure, leading to right-angle components (local motifs) resembling (similar to) those in the crystalline counterpart of this chalcogenide glass. The dominance of p bonding is revealed by (i) distributions of the coordination number (CN) and the bond angle, for truly bonded atoms determined based on the electron localization function, and (ii) a direct evaluation of the p (and s) orbital occupation probability for the CN=3 Ge atoms that form 90 degree bonds with neighbors. These structural features may have implications for the rapid crystallization and poor GFA of the GST.

B01

Mathematical Modeling: an efficient way to predict inclusion evolution in liquid steel

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Despite continuous improvement, harmful inclusion elimination in liquid steel remains a challenge for steelmaking industry, since a lot of defects observed on hot or cold products are directly linked with difficulties to eliminate inclusions at different stages of the elaboration process. This is why ArcelorMittal R&D has decided to develop some predictive tools, which can deal with physico-chemistry aspects for inclusion precipitation, and with fluid mechanics for inclusion transport. The paper first presents the development of models for the prediction of alumina formation in liquid steel bath. The process of aluminum melting in liquid steel is investigated, by means of multiphase CFD (Computational Fluid Dynamics) model. To predict alumina formation, coupling between thermodynamics and CFD is performed. This coupling is a key tool for deoxidizing optimization, making possible a "rapid" study on influence of geometrical parameters of reactor, size of deoxidizers, recirculating flow rate… Kinetics for inclusion formation can also be assessed, but difficulties are encountered when both inclusion size and composition should be predicted simultaneously. The paper gives some insight into the physical modeling, the coupling with thermodynamics and the numerical procedure which was developed and implemented in a CFD package, based on the so-called multi-QMOM, to get the size distribution with an acceptable effort from a computer point of view.

B02

Recrystallization kinetics of austenite in Nb microalloyed steel

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The knowledge of the relationship between the thermomechanical conditions and the final microstructure and properties of a steel product, often requires a strong interaction between numerical models and experimental data. In this paper, hot strength and recrystallization kinetics of austenite in a Nb microalloyed steel were experimentally investigated by single and double hot compression tests, varying the strain rates and the deformation temperatures. For comparison a plain carbon steel was studied by the same procedures. The effects of deformation temperature, strain rate and addition of Nb on peak stress and softening/ recrystallization fractions of the materials were assessed. The data obtained from the mechanical tests were compared with the results obtained from the metallographic analysis revealing the prior austenitic boundaries and measuring the grain size distribution. Finally, the comparison between the mechanical and metallographic method allowed a better interpretation of the results obtained from the classical double hot compression tests.

Keywords: *Recrystallization; double hot compression tests; metallography; hot deformation.*

B03

Computation of the Isothermal Transformation Diagrams of 42CrMo4 Steel from the Dilatometer Measurements with Continuous Cooling

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To generally predict the mechanical properties of steels following heat treatment, the isothermal time-temperature-transformation (TTT) diagrams must be known. The isothermal kinetics of the phase transformation is influenced by the austenitisation conditions and the deformation processes. Due to the requirements of the process chain "integrated heat treatment following hot-forging", the steels are austenitised at a comparatively high temperature and deformed before quenching. The TTT diagrams found in the literature only treat limited austenitisation temperatures and do not generally consider different deformation levels. However, the measurements of the corresponding TTT diagrams are both costly and time consuming. In addition to this, the isothermal transformations of low alloyed steels, which transform very quickly, can not be measured using those dilatometers which are readily available [1]. In this paper, the TTT diagrams of the 42CrMo4 steel austenitised at 1200°C and deformed at different levels are computed from the dilatometer measurements with continuous cooling using the methods developed by Buza [2] and Rios [3].

Keywords: *TTT diagram, dilatometer measurement, integrated heat treatment, Buza, Rios, 42CrMo4*

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B04

Prediction of Microstructure and Mechanical Properties in Aluminum Castings after Heat Treatment

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A comprehensive numerical model is being developed for the calculation of the final microstructure and mechanical properties of aluminum casting alloys after heat treatment. After specifying the alloy chemical composition, solidification process, and heat treatment parameters, the model predicts the microstructure and potential defects through various stages of the component lifecycle: casting, solid solution heat treatment, and artificial aging. The calculation is chained such that the resultant microstructure of the previous event, such as casting, is used as the initial condition of the following event, ensuring the tracking of the component history and maintaining a high level of accuracy across metallurgical stages. The model takes into account the relationship between the different input parameters and the link to basic metallurgical features. Such a model can be used for tailoring mechanical properties and component performance with the correct choice of chemical composition and manufacturing process parameters. The effects of cooling history during casting

and heat treatment processes on aluminum alloy castings are numerically and experimentally investigated. The microstructure and mechanical properties are predicted and compared with experimental measurements.

Keywords: *Aluminum casting, heat treatment, modeling, mechanical properties, mcirostructure*

B05

Size-dependent lognormal grain size distribution in nanocomposite films

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A key challenge in nanocomposite films with nanostructures comprising of nanocrystalline (nc) phase surrounded by an amorphous (a) matrix is controlling grain size and its distribution. We report a size-dependent lognormal grain size distribution (GSD) in nanocomposite films by using high resolution transmission electron microscopy. Monte Carlo simulations reveal that the homogenous and inhomogenous grain growth modes are decided by the different energy exerted on each grain boundary (GB) and diffusion-controlled processes with different grain sizes, leading to lognormal and off-lognormal GSDs, respectively. The results also indicate that the lognormal GSD of the system has the microstructure which attains to the percolation threshold with the smallest grain size dispersion and the longest GBs.

Keywords: *Monte Carlo simulations, Nanostructure, Grain size distribution*

B06

Modelling Hydrogen Diffusion and Phase Transformation for Titanium Powder Hydrogenization-Dehydrogenization (HDH) Rolling Process

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Titanium-based products are generally characterized by high manufacturing costs due to the poor machinability of the materials. Due to the poor machinability, machining of titanium and its alloys would always be a problem. An alternative method that has the potential to become a cost-effective method for manufacturing titanium-based components is the powder metallurgy, because it can produce near-net-shape parts. A potential method that could further reduce the manufacturing costs of the powder metallurgy products is the induction of hydrogen to reduce the hardness of titanium particles and the subsequent removal of hydrogen to restore the performance of the products.

Charging with an appropriate amount of hydrogen can remarkably improve the mechanical properties of titanium alloys, due to the effect of hydrogen, as an alloying element, on phase compositions, development of metastable phases and kinetics of phase transformations. The induced hydrogen can reduce the resistance to deformation, improve the forming property and refine the grain of titanium alloys. As a result, the powder metallurgy can be conducted under lower forming load and fabricate high-quality parts to close tolerance at low cost. Due to a positive enthalpy of solution of hydrogen in titanium, the reaction of hydrogen with titanium is reversible, which allows hydrogen to be easily removed from titanium products by vacuum annealing, before they are used, to prevent hydrogen-related failures in service. In the thermohydrogen processing of titanium alloys, hydrogen as a temporary alloying element diffuses in the titanium allays, leading to the phase transformation and microstructure evolution and, sequentially, the change of mechanical properties. Therefore, the study of quantitative hydrogen diffusion and phase transformation behavior in titanium alloys is significant to improve the understanding of the effect of hydrogen on the machinability of titanium components and for the development and application of the powder metallurgy of titanium.

In this paper we studied the processes of phase transformation and diffusion of hydrogen in titanium particles by computational thermodynamics simulation, focusing on the simulation of hydrogen diffusion between titanium particles and in the components produced by compacting titanium powder, especially the diffusion process in titanium particle packages at different temperatures. The hydrogen diffusion and the growth of different titanium phases at different thermo-hydrogen processing temperatures were analyzed quantitatively. The simulation provides fundamental data for titanium powder HDH process.

Keywords: *hydrogenation, dehydrogenation, diffusion, phase transformation, thermodynamics modeling, titanium powder*

B07

Modeling for prediction of carbide formation and dissolution in vacuum carburization process

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Carbide has a big influence on the quality of carburized parts, especially for the vacuum carburization process in which the carbon flux across the surface may be larger than atmosphere carburization. In this paper a model has been developed to predict the formation and dissolution of carbide based on the diffusion and phase equilibrium for the multi-pulse vacuum carburization process. The result shows the procedure about the generation, growth and fade of carbide, which will help to determine the process parameters for the optimal performance.

Keywords: *Modeling, carbide formation, diffusion, phase equilibrium, vacuum carburization*

B08

The formation of nanometer coherent structures during spinodal decomposition and ordering coexistence phase transformation in Fe-24Al alloys

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The nanometer coherent structures evolution of spinodal decomposition and ordering coexistence phase transformation in Fe-24Al alloys is investigated by the microscopic phase field kinetic model. The results show that the concentration and long-range order parameters all continuously changes towards to their equilibrium values during phase transformation. With the increase of elastic interaction energy, the anisotropy along [01] or [10] elastic soft direction is more obvious and the time reaching equilibrium state is also shortened. According to the results, the formation of nanometer coherent structures during phase transformation is composed of the initial decreasing stage of order degree stage, the incubation stages, the continuous increasing stage of concentration order parameter and long-range order parameter, and the later stable stage. The spinodal decomposition and ordering is interaction, the initial ordering stage is the necessary condition of the coexistence phase transformation. The nanometer coherent structures are not found to grow during the whole phase transformation. The simulation results are in accord with the results in experiment obtained by the aging treatment in Fe-24Al alloys.

Keywords: *spinodal decomposition; ordering; coherent structures; phase field*

b09

Study on the initiation and evolution of strengthening phase in niobium micro-alloyed steel by 3DAP

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It is of great significance to study the initiation and evolution of strengthening phase, because it plays an important role in determining the mechanical properties of materials. In this paper, three dimensional atom probe (3DAP) was used to characterize the composition, sizes, distribution and evolving rules of clusters, that is strengthening phase in the early stage in niobium micro-alloyed steel solution treated and aged with different conditions. Results showed that clusters with a few nanometers have a plate-like morphology, which initiated at 700℃ within 5 minute and stopped participating about 30 minutes. Interstitial atom in the clusters segregated fast than substitional atom at early clustering process. Related theories were also discussed.

Keywords: *Micro-alloyed steel; 3DAP; Strengthening phase; Solution treating and aging.*

B10

Calculation on the Incubation Period of Proeutectoid Ferrite Transformation for Si-Mn Trip Steel

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The incubation period of proeutectoid ferrite transformation for Si-Mn TRIP steel has been calculated by using Aaronson’s incubation period model for transformation. The influences of chemical compositions and hot deformation of austenite on incubation period have been taken into consideration in the calculation, and some parameters have been proposed and validated with the measured time temperature transformation (TTT) curves from dilation tests. The calculation results show that it is essential to take into account of the effect of solute atoms on the interfacial energy in austenite grain boundaries. For hypoeutectoid steel, the incubation period of ferrite transformation increases with the increase of C and Mn contents, and C has a greater impact than that of Mn, while the incubation period of ferrite transformation decreases with the increase of Si content. Hot deformation shortens the incubation time and promotes austenite to ferrite transformation.

Keywords: *TRIP steel, proeutectoid ferrite, phase transformation, incubation period*

b11

Modelling of nucleation and growth of $M_{23}C_6$ carbidein multi-component Fe-based alloy

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Three-dimensional atom probe (3DAP) technique has been used to study the nucleation and growth of M23C6 carbide in a supersaturated multi-component Fe-based alloy aged at 800℃. 3D images indicate that the radius of M23C6 carbide after ageing for 10 min is about 9 nm. Concentration profiles of alloy elements

in the carbide are also obtained. Combined with PANDAT and Thermo-Calc software, attempts to model the early stages of precipitation are present. The calculated particle size and composition of M23C6 carbide is in good agreement with 3DAP data.

Keywords: *Nucleation and growth, M23C6, 3DAP*

B12

Experimental Study of Bainite Transformation Plasticity during Continuous Cooling for Armour Steel

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Transformation plasticity is inverse deformation during phase transformation under low loading. During the welding and quenching of armour steel, accompanying with the complicated thermo-mechanics processes, Bainite transformation plasticity has great influence on the distortion and distributing of the residual stress in workpiece, so it is essential to research the bainite transformation plasticity during continuous cooling. By applied varied uniaxial load, an experimental method of determined bainite transformation plasticity of materials is introduced. The total strain was decomposed by considering elastic strain, thermal strain, metallurgical strain and bainite transformation plasticity strain, then the bainite transformation plasticity strain were gained. Moreover, the quantity law for bainite transformation plasticity strain of materials under different applied load and temperature was yielded. These results can provide a method for research the thermal-mechanics behavior of armour steel during heat treatment or welding.

Keywords: *Transformation plasticity, Bainite transformation, Continuous cooling, Armour steel*

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B13

A general approach on the order-disorder transition of complex intermetallics by combining thermodynamic model with first-principles calculations

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The ordering behaviours of the alloying elements in intermetallics are of fundamental and technical importance. A general approach by combining thermodynamic model with first-principles calculations was developed. The quantitative relationship among the site occupying fraction of the constituent elements vs. alloy composition and temperature were studied theoretically without referring experimental data as input. The general approach is not limited by the complexity of composition, structure and the character of the phase transition. Currently we predicted the ordering behaviors of many types of intermetallics with multi-components in a considerable accuracy, such as Ti_2AlNb-based orthorhombic phase with Ta, W, Cr, V, Zr additives, AB_2-C15 multi-component Laves phase, $ThMn_{12}$-type $YFe_{10}Mo_2$

with Si, Co additives and multi-component A_3B-$L1_2$ phase. The predicted results are explored further to guide the alloy design. In this contribution, the detail of the sublattice model and the mathematical algorithms were given in detail. Some predicted results and their application in alloy design were reported.

The sublattice model is shown in equation (1), where W_j is sublattice denoted with Wyckoff position, $y_{E_i}^{W_j}$ is site occupancy fraction of species E_i on sublattice W_j. f_{W_j} is fraction of sublattice W_j.

$$\left(E_1 y_{E_1}^{W_1}, E_2 y_{E_2}^{W_1}, \cdots, E_i y_{E_i}^{W_1}\right)_{f_{W_1}} \left(E_1 y_{E_1}^{W_2}, E_2 y_{E_2}^{W_2}, \cdots, E_i y_{E_i}^{W_2}\right)_{f_{W_2}} \cdots \left(E_1 y_{E_1}^{W_j}, E_2 y_{E_2}^{W_j}, \cdots, E_i y_{E_i}^{W_j}\right)_{f_{W_j}} \quad (1)$$

The selective results of site fractions with temperature are shown in Fig 1.

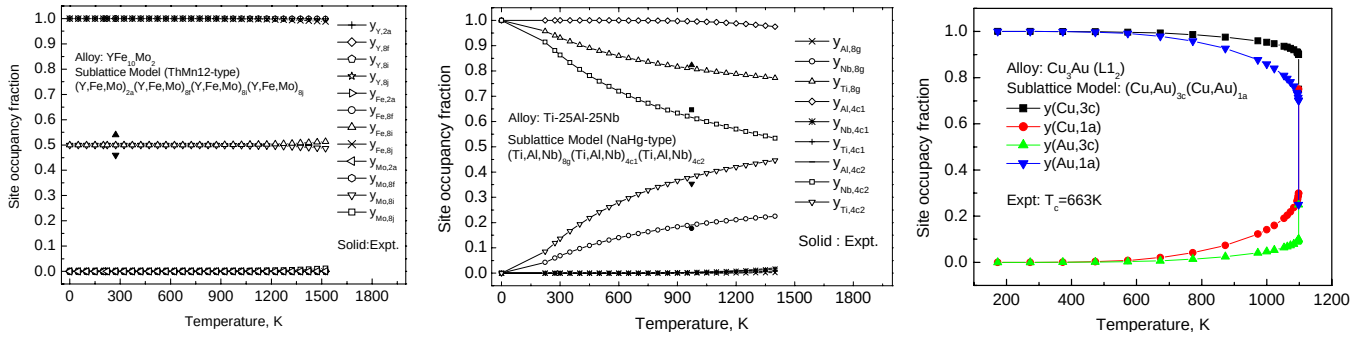

Fig 1. The plots of site occupancy fraction of alloying elements vs. temperature in different kind of intermetallics, the results show that the general approach can deal with diverse types of order-disorder transition in multi-component intermetallics.

Keywords: *Intermetallics,* Order-disorder transition*, Sublattice modeling, First-principles calculations*

B14

First-principles investigation of the structural stability and electronic property of precipitates on the Cu-rich side of Cu-Ni-Si alloys

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The energetic and electronic structures of precipitates on the Cu-rich side of Cu-Ni-Si alloys were investigated by using first-principles calculations based on plane-wave pseudopotential method. The negative formation heats and the cohesive energies of these precipitates were estimated with electronic structure calculations, and their structural stability was also analyzed. The results show that δ-Ni2Si, γ-Ni5Si2 and β-Ni3Si precipitates all have great alloying ability and structural stability, which, after comparing their density of states (DOS), is found attributed to the pseudogap effect near the Fermi level (EF) and strong hybridization between the Ni-3d and Si-3p states. Compared with the other two precipitates, the δ-Ni2Si precipitate has the greatest structural stability, which is resulted from its lower DOS at EF and the main bonding peaks slightly moving to the low energy region.

Keywords: *precipitate; first-principles; electronic structure; structural stability*

B15

Prediction of the site occupancies of alloying elements in D019-type Ti3Al-based alloy by combining thermodynamic model with *ab initio* calculations

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Ti_3Al-based alloy has potential applications in aerospace due to its high specific strength and good oxidation resistance at elevated-temperature. However, its poor ductile properties hamper its application economically. Adding ternary or quaternary alloying elements is proved to an effective way to improve it comprehensive properties. In this contribution, the site occupancies of V, Cr, Ga, Sn, Mn, Zr, Nb, Mo, Ta, and Zn in $D0_{19}$-type Ti_3Al-based alloys with different compositions are predicted by combining thermodynamic model with *ab initio* calculation. The sublattice model is shown in equation (1), where *c* and *h* are sublattices denoted with Wyckoff position, 2 and 6 are the multiplicity, which correspond the relative fraction of sublattice *c* and *h*, respectively.

$$\left(E_1 y_{E_1}^{2c}, E_2 y_{E_2}^{2c}, \cdots, E_i y_{E_i}^{2c}\right)_{2c} \left(E_1 y_{E_1}^{6h}, E_2 y_{E_2}^{6h}, \cdots, E_i y_{E_i}^{6h}\right)_{6h} \quad (1)$$

The predicted results show that Ga and Sn atoms occupy Al sites (2c), while V, Cr, Mn, Zr, Nb, Mo, Ta and Zn atoms occupy Ti sites (6h). It is also predicted that the alloys composition have no significant influence on their site preference. The site occupation of elements in alloys is weakly dependent on temperature. Quantitative agreement between the predicted results and reported experimental results is reached. Comparing with the study in literature referring to special supercell, the model employed in this contribution is not limited by the number of component and the alloy composition. More than three alloying elements contained in the same alloy can be calculated easily.

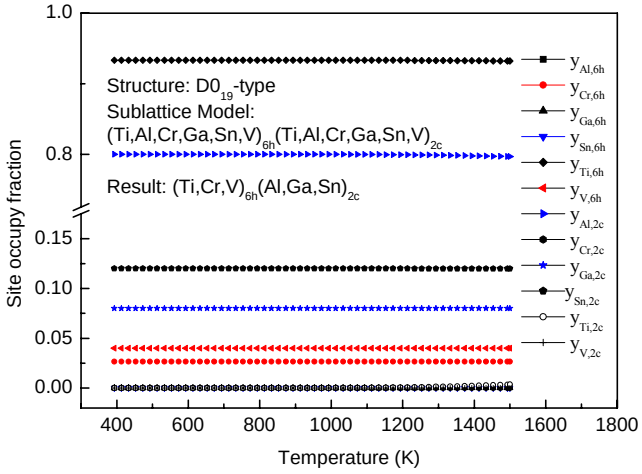

Fig. 1 The predicted results of the Ti-20Al-2Cr-2Ga-3Sn-3V alloy

Keywords: *Ti3Al-based alloy, Site occupancy, Ordering behaviours, Sublattice modeling, Ab initio calculations*

B16

First-principles calculation of the temperature dependence of hardening precipitation in Mg-Gd alloys

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First-principles thermodynamic models based on the cluster expansion formalism, lattice dynamics calculations and quantum-mechanical total energy calculations are employed to compute the metastable hardening precipitation in hcp-based α-Mg-Gd alloys. We show that vibrational entropy reverses the energetic preference, and plays a critical role in the hardening precipitation at different aging temperatures in Mg-Gd alloys. In addition to energetics, the analysis of bonding charge density reveals that the metastable β′ phase is responsible for the high strength during subsequent isothermal treatment. Our results are found to be in good agreement with experimental measurements and help clarifying the metastable precipitation sequence in Mg-Gd alloys.

Keywords: *First-principles calculation, Mg-Gd alloys, precipitation*

B17

Prediction of the site occupancy of alloying elements in REFe12-xMx-based alloy with ThMn12 prototype by combining thermodynamic model with first-principles calculations

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$REFe_{12-x}M_x$-based alloy with $ThMn_{12}$ prototype has potential applications as advanced magnetic properties. Adding ternary or quaternary alloying elements is proved to an effective way to improve it comprehensive properties. In this contribution, the site occupancies of RE (RE=rare earth elements), Fe, and M (M=Mo, Si, Ti, Co) with different compositions are predicted by combining thermodynamic model with first-principles calculations. The sublattice model is shown in equation (1), where *a*, *i*, *j* and *f* are sublattices denoted with Wyckoff position, 2, 8, 8 and 8 are the multiplicity, which correspond the relative fraction of sublattice *a*, *i, j* and *f* , respectively.

$$\left(E_{1}{}_{y_{E_1}^{2a}}, E_{2}{}_{y_{E_2}^{2a}}, \cdots, E_{i}{}_{y_{E_i}^{2a}}\right)_{2a}\left(E_{1}{}_{y_{E_1}^{8i}}, E_{2}{}_{y_{E_2}^{8i}}, \cdots, E_{i}{}_{y_{E_i}^{8i}}\right)_{8i}\left(E_{1}{}_{y_{E_1}^{8j}}, E_{2}{}_{y_{E_2}^{8j}}, \cdots, E_{i}{}_{y_{E_i}^{8j}}\right)_{8j}\left(E_{1}{}_{y_{E_1}^{8f}}, E_{2}{}_{y_{E_2}^{8f}}, \cdots, E_{i}{}_{y_{E_i}^{8f}}\right)_{8f} \quad (1)$$

The predicted results show that the site occupying preference of the alloying elements RE are always tend to occupy the 2*a* sublattice, Fe atoms tend to prefer 8*f* and 8*j*, and 8*i* sublattices are shared by Fe and transition metals or Si. The site occupations of elements have no change with the increase of the temperature. The results agree well with the limited reliable experiments.

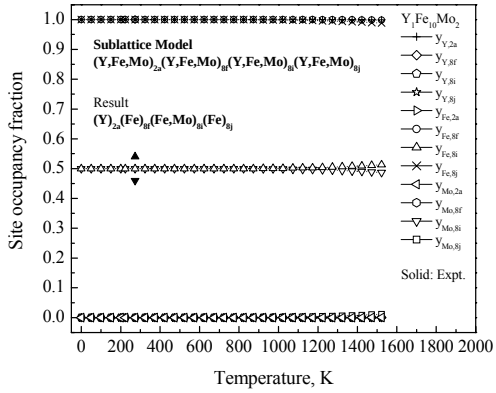

Fig. 1. The site occupancy fractions of elements in sublattices vs. temperature of the stoichiometric intermetallics $YFe_{10}Mo_2$ with experimental data [5] superimposed.

Keywords: *Rare earth magnetic materials, Site occupancy, Thermodynamic modeling, First-principles calculations*

B18

Prediction of the site occupancy of alloying elements in Ni3Al-based L12 alloy by combining thermodynamic model with first-principles calculations

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Ni_3Al-based alloy has potential applications in aerospace due to the positive temperature-dependence of its yield strength as well as its good oxidation resistance at elevated-temperature. In order to match the high requirement for the specific strength and enough ductile in modern aeroengine, adding ternary or quaternary alloying elements is proved to an effective way to improve it comprehensive properties. In this contribution, the site occupancies of more than twenty alloying elements with different compositions are predicted by combining thermodynamic model with First-principles calculations. The sublattice model of the $A_3B\_L1_2$ is shown in equation (1)

$$\left(E_{1y_{E_1}^{3c}}, E_{2y_{E_2}^{3c}}, ..., E_{iy_{E_i}^{3c}}\right)_{3c}\left(E_{1y_{E_1}^{1a}}, E_{2y_{E_2}^{1a}}, ..., E_{iy_{E_i}^{1a}}\right)_{1a} \quad (1)$$

where *a* and *c* are sublattices denoted with Wyckoff position, 1 and 3 are the multiplicity, which correspond the relative fraction of sublattice *a* and *c*, respectively.

The predicted results agree well the limited reliable experimental and theoretical results. Compare with the literature, our model can predict the site occupancies of multi-components contained in the same Ni_3Al-based alloy easily, which means we can consider the complex interaction of the alloying elements.

Keywords: *Ni_3Al-based alloy, Site occupancy, Thermodynamic modeling, First-principles calculations*

B19

Prediction of the ordering behaviours of alloying elements Ta, V, Mo and Hf in Ti2AlNb-based orthorhombic alloy by combining thermodynamic model with ab initio calculations

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Ti_2AlNb-based orthorhombic alloy has potential applications in aerospace due to its high specific strength and good oxidation resistance at elevated-temperature. However, its poor ductile properties hamper its application economically. Adding ternary or quaternary alloying elements is proved to an effective way to improve it comprehensive properties. In this contribution, the site occupancies of V, Cr, Ta, and Hf with different compositions are predicted by combining thermodynamic model with *ab initio* calculation. The sublattice model is shown in equation (1), where *g*, c1 and *c2* are sublattices denoted with Wyckoff position, 8, 4 and 4 are the multiplicity, which correspond the relative fraction of sublattice *g*, *c1* and *c2*, respectively.

$$\left(E_1 y_{E_1}^{8g}, E_2 y_{E_2}^{8g}, \cdots, E_i y_{E_i}^{8g}\right)_{8g} \left(E_1 y_{E_1}^{4c1}, E_2 y_{E_2}^{4c1}, \cdots, E_i y_{E_i}^{4c1}\right)_{4c1} \left(E_1 y_{E_1}^{4c2}, E_2 y_{E_2}^{4c2}, \cdots, E_i y_{E_i}^{4c2}\right)_{4c2} \quad (1)$$

The predicted results show that the site occupying preference of the alloying elements V and Hf is similar with Ti, and the Mo and Ta is similar with Nb. The alloys compositions have no significant influence on the site preference of Al atoms. The ordering behaviour of Ti_2AlNb is stronger than Ti_2AlTa, which support the result that the ductile of Ti-22Al-20Nb-7Ta is larger than Ti-22Al-27Nb. The site occupation of elements except Al in alloys change continuously with temperature, which means there is a second-order character concerning with the order-disorder transition. Quantitative agreement between the predicted results and limited experimental data is reached. The model employed in this contribution is not limited by the number of component and the alloy composition. Multi-components contained in the same alloy can be calculated easily.

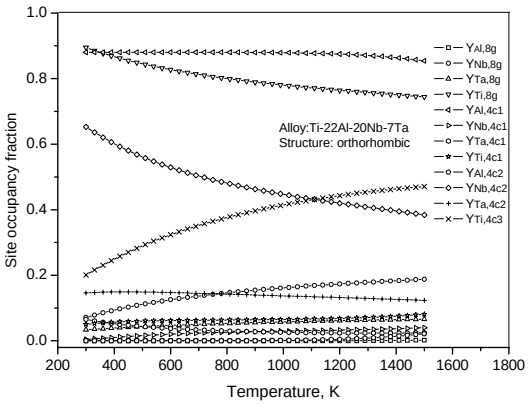

Fig. 1 The predicted results of the Ti-20Al-20Nb-7Ta alloy

Keywords: *Titanium Aluminum alloy, Site occupancy, Ordering behaviours, Sublattice modeling, Ab initio calculations*

B20
The heat treatment of superbainitic ferrite

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Superbainitic steels with an extraordinary combination of ultrahigh strength and excellent toughness have been drawn much attention, and become the prospective armour material. These properties are achieved by designing superbainitic steels, with high-silicon and high-carbon composition, such that the transformation to bainite can be conducted at a much lower temperature than usual, resulting in the very fine bainitic plates and the fine scale dispersion of austenite between the plates. It's worth intention to design new alloy-steels using the theory of bainite reaction, for creating this new class of ultrahigh strength steels.
The objective of this work was to investigate the superbainitic structures in two experimental high-silicon

and high-carbon steels, with 5 and 24 ppm levels of boron, separately. After austenitization, the specimens of the steels were held at three different isothermal transformation temperatures (150, 200 and 300℃) for a variety of time intervals. The microstructures have been examined via optical metallography (with microhardness measurement) and transmission electron microscopy. It was found that after isothermal transformation at 200℃ for 10 days, both steels could produce a high volume fraction of sheaf structures with nanometer-scaled bainitic ferrite subunits, which contributed to an ultrahigh microhardness, up to HV 690. In this paper, the nano-structural details and the transformation characteristics of the corresponding specimens isothermally treated at 150, 200 and 300℃ will be presented.

Keywords: *Superbainitic steels, low-temperature isothermal transformation, Vickers hardness, transmission electron microscopy*

B21

Microstructure Design and Implementation of New Generation High Strength Multi-phase Steels

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In this paper, the strategy for designing optimal microstructure of new generation advanced high strength steels (AHSS) for automobiles has been reviewed. The main concerned factors include medium carbon content, low alloying elements and lower cost of adequate processing for new affordable AHSS. The multi-phase microstructure consisting of hard phase matrix, fine inherited soft phase and nano-sized precipitate (coherent or semi-coherent) seems promising for the new generation AHSS. Three different processes (quenching and partitioning, quenching-partitioning-tempering and quenching-partitioning-austempering) have been practiced to obtain an optimal microstructure, which are made up of martensitic matrix (hard phase), retained austenite slides/films (soft phase), and nanocarbide/ nanobainite.

Keywords: *High strength multi-phase steels; Martensite; Retained austenite; Nano-sized precipitate; Nanobainite*

B22

Design of high entropy alloy with FCC structure by combining thermodynamic model with first-principles calculations

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High-entropy alloys are promising alloys that are composed, by definition, of at least five principal elements with concentrations in the range of 5–35 *at.*%. The high-entropy alloys tend to form simple solid solution phases mainly of cubic crystal structure, especially at elevated temperatures. A new approach for the design of alloy systems with multiprincipal elements is contributed based on a kind of reversed thinking that the alloy elements in high entropy alloy tend to be disordered on the sublattice of the corresponding intermetallics. We use a general approach by combining thermodynamic model with *ab initio* energetic calculation on end-members to predict the site occupying tendencies of the alloying elements in intermetallic compound $A_3B\_L1_2$ (It becomes a face-centered cubic structure, when A and B

are the same element), a set of compositions for high entropy alloy are proposed. Currently, we finished the calculation on the system including the following 19 alloying elements, i.e., Ag, Al, Au, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Pb, Pd, Sb, Sn, Ti, V, W, Zr. The suggested high-entropy alloy constituents are Sn, Au, Cr, Ti, Ni, Sb, and Fe. The candidate elements are being still extended. The sublattice model of the $A_3B\_L1_2$ is shown in equation (1), where W_1 and W_2 is sublattice *a*, *c* , $y_{E_1}^{W_1}$ is the site fraction of element *i* on sublattice *j*.

$$\left(E_1 y_{E_1}^{W_1}, E_2 y_{E_2}^{W_1}, \ldots, E_i y_{E_i}^{W_1}\right)_{3c} \left(E_1 y_{E_1}^{W_2}, E_2 y_{E_2}^{W_2}, \ldots, E_i y_{E_i}^{W_2}\right)_{1a} \quad (1)$$

The predicted relationship of site fractions with temperature is shown in Fig 1.

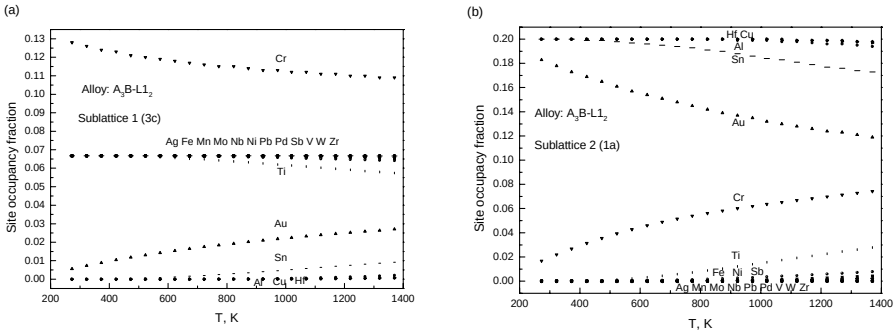

Fig. 1 The site occupancy fractions of the alloying elements in the sublattices of the $Cu_3Au\text{-}L1_2$ phase with 19 alloying element Ag, Al, Au, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Pb, Pd, Sb, Sn, Ti, V, W, and Zr. Except x_{Cr} =0.1 mol, the content of the rest 18 elements is 0.05, respectively. From the map of the site occupancy fraction, we recommend the high-entropy alloy (tend to as disordering as possible) constituents to be Sn, Au, Cr, Ti, Ni, Sb, and Fe.

Keywords: *High-entropy alloy, site occupancy, Thermodynamic modeling, First-principles calculations*

B23

Design of magnetic high entropy alloy with FCC structure by combining thermodynamic model with first-principles calculations

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Magnetic high-entropy alloys are of great interesting due to the special mechanical properties and acceptable magnetic properties. In this paper, based on a magnetic high entropy patent with composition system (Fe, Co, Ni, Mn, Bi, Tm), we extend the compositions choice by considering the site occupancy of a series alloying elements on the two sublattice 3c and 1a in $Cu_3Au\text{-}L1_2$ prototype. We first consider the candidate elements for high entropy alloy if the alloying elements tend to be disordered on the sublattices, and then we choose the system containing magnetic atoms Fe, Co, and Ni. More than 5 sets of candidate compositions are recommended as magnetic high-entropy alloys. The candidate elements are being still extended. The sublattice model of the $A_3B\_L1_2$ is shown in equation (1), where W_1 and W_2 is sublattice *a*, *c*, $y_{E_1}^{W_1}$ is the site fraction of element *i* on sublattice *j*.

$$\left(E_1 y_{E_1}^{W_1}, E_2 y_{E_2}^{W_1}, \ldots, E_i y_{E_i}^{W_1}\right)_{3c} \left(E_1 y_{E_1}^{W_2}, E_2 y_{E_2}^{W_2}, \ldots, E_i y_{E_i}^{W_2}\right)_{1a} \quad (1)$$

Keywords: *High-entropy alloy, Magnetic materials, Ordering behaviours, Thermodynamic modeling, First-principles calculations*

B24

Predicting the CCT Diagrams of Steels Using Artificial Neural Network Models

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Eagleye2003__a computer software for predicting the continuous cooling transformation(CCT) diagrams of novel air-cooled bainite steels was developed in this paper. Artificial neural network models in Eagleye2003 were trained. CCT diagrams of four novel air-cooled bainite steels were predicted using Eagleye2003. The prediction results showed that the prediction performance of the software is satisfactory. It is helpful to the prediction of microstructure and properties and alloy design of steels.

Keywords: *CCT diagrams, Artificial neural network, Eagleye2003, Predict*

B25

The reconstruction of the temperature field base on Matlab and two-dimensional interpolation

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This study, based on the two-dimensional interval B-spline interpolation, reconstructs the temperature distribution rapidly on the basis of the existing actual measurement data in Matlab, processes and outputs images, so as to reflect the overall temperature distribution to timely control the temperature of heating equipment.

Keywords: *the temperature field reconstruction, spline function, value computation, two-dimensional interpolation*

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b26

Process of Equiaxed Grains of RE-Al Alloy under Slope Vibration

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A new technique using slope vibration casting process during heating and isothermal holding period to prepare Al-7Si-2RE alloy has been studied. The small, near-spherical and non-dendritic microstructure with the semi-solid processing requirements has been obtained. Experiments show that the cooling method, pouring process and the convection of melt caused by slope vibration had significant effects on the formation of near-spherical primary gains. The water-cooled copper mold casting with slope vibration at the temperature near liquidus can obtain Al-7Si-2RE alloy with small homogeneous equiaxed grains, the average grain diameter is 48.3μm, and the average grain roundness is 1.92.

Keywords: *convection; slope vibration; equiaxed grains; rare earth elements; solidification curve*

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b27

Calculation on the solid solution forming enthalpies of Re-Mo-Ti Gradient alloy in thermodynamics

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The idea about preparation of Re-Mo-Ti alloy was put forward because of applications of Re and Mo-Re alloy in aerospace. Basing on thermodynamics theory, the feasibility of developing a new high temperature alloy Re-Mo-Ti was investigated. The solid solution forming enthalpies of binary alloy Re-Ti, Mo-Ti, Mo-Re were calculated with Miedema thermodynamics theory. The Miedema theory of binary alloy could be used in ternary alloy through Kohler model or Toop model. The calculated results show that forming enthalpies of binary alloy Re-Ti, Ti-Mo and Re-Mo are negative, which indicate that binary alloy Re-Ti, Ti-Mo and Re-Mo could form solid solution among wider component area. The forming enthalpies of Ti–Mo-Re ternary alloy are still negative and smaller than that of binary alloy Re-Ti, Ti-Mo or Re-Mo, which indicates it is possible to form large solid solution graph area among ternary alloy of Ti, Mo, Re element. It is feasible to develop a new high temperature material in thermodynamics, in this material

Ti–Mo-Re solid solution as base phase, and the Ti_5Re_{24} intermetallic compounds or ω phase as strengthening phase.

Keywords: *Re-Mo-Ti alloy, Gradient materials, Solid solution forming enthalpy, Thermodynamics*

b28

Monte Carlo study of B2-$L2_1$ ordering transitions in Au-Cu-Al systems

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The B2-L21 ordering transitions in Au-Cu-Al shape-memory alloys were studied by Monte Carlo exchange simulations, where a set of first, second and third nearest-neighbors mixing potentials for Cu-Al in the Au-Cu-Al alloys were calculated from first principles using the Connolly-Williams method. To ensure the phase stability of the β-Au-Cu-Al, the investigation includes the range of compositions $Au_2Cu_{1-x}Al_{1+x}$ ($-0.15 \leq x \leq 0.15$). The B2-$L2_1$ transition temperatures were predicted, which were in agreement with the experimental results, and the atomic ordering around the vacancy of the $L2_1$ structure was further discussed.

Keywords: *Au-Cu-Al alloys, B2-$L2_1$ transitions, Monte Carlo simulation, vacancy*

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b29

Numerical simulation of temperature distribution and heat transfer during the solidification of Ti-6Al-4V ingots in VAR process

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During the Vacuum Consumable Arc Remelting (VAR) process, temperature distribution and heat transfer between the molten metal and the crucible have a significant effect on the solidified structure and mechanical properties of cast ingots [1, 2]. Here, in order to get a better understanding of the VAR processes and thus to optimize them, a 3D finite element model is developed for the temperature fields and heat transfer of Ti-6Al-4V ingot during VAR process by ANSYS software. The results show that the temperature fields obtained by the simulation are well validated through the experiment results. The temperature distribution is different during the whole VAR process and the steady-state molten pool has formed at 329s. At the initial stage of remelting, the heat dissipation of crucible bottom plays an important role in the whole heat dissipation system; At the middle of remelting, the crucible wall becomes a major heat dissipation way. In the end, the effect of cooling velocity on the solidification structure of ingots is investigated based on the temperature fields and the results can well explain the macrostructure differences of Ti-6Al-4V ingots.

Keywords: *VAR process; titanium alloy; solidification; temperature fields; heat transfer*

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b30

Numerical Simulation of Temperature and Stress Fields in Beryllium Cutting Process

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The temperature and stress fields in beryllium during high speed cutting process were studied by employing a thermo-mechanically coupled finite element method (FEM). The results show that the cutting temperatures in beryllium increase only a little. Both of the residual stresses for parallel and vertical to the cutting direction are tensile stresses in the surface of beryllium after cutting. The cutting force and thrust force are about

280N/mm and -250N/mm during the steady cutting stage, respectively. The main effects of coolant on the cutting process are to decrease the friction coefficient and heat between the tool and the workpiece, then reduce temperature, but almost no effects for stress. This study is helpful to enhance the understanding for stress formation and optimizing the process parameters of beryllium.
Keywords: *Beryllium, temperature field, stress field, cutting, FEM*

B31

Microstructural evolution of two way hysteresis-free shape memory effect in Mn-based antiferromagnetic alloys

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This paper reports the microstructural evolution of two-way hesteresis-free shape memory effect in Mn-rich antiferromagnetic alloys with three-dimensional phase field model. The results show that forward martensitic twins are grown up with decreasing temperature and shrunken with increasing temperature. It is proved that the relaxation of stored strain energy during the forward martensitic transformation plays a key role when reverse martensitic transformation takes place.

Keywords: *Microstructural evolution; Phase field model; Computer simulation; Two-way shape memory effect*

B32

The effects of coherency stress on interdiffusion across coherent multilayer interfaces

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Interdiffusion across coherent interfaces in nanoscale multilayered films is studied, focusing on the effects of the coherency stress on the diffusion of the vacancy and the component species, and on the effects of the vacancy concentration on the diffusivities of the component species. Two situations are considered: (1) Vacancy source is assumed to exist only on the surfaces, therefore the model explicitly accounts for the diffusion of the vacancy and the two component species; (2) vacancy sources such as dislocations and grain boundaries are assumed to exist within the layers, and concentration of vacancy is assumed to be in the equilibrium state as a function of local stress field, therefore the model only explicitly accounts for the diffusion of the two component species. For simplicity, the coherency stress field is calculated from the distribution of the two component species. The diffusion dynamics of these two cases, along with that without considering the effects of the coherency stress, are compared. It is found that coherency stress may

greatly suppress or enhance the diffusion process, depending on the intrinsic diffusivity and the atomic volumes of the species, and case (1) has a more profound effect than case (2).

Keywords: *interdiffusion, stress effect, multilayer*

b33

Simulating mechanical behaviour of porous materials for SOFC

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In the study, periodic homogenization method was adopted to predict the micro-scale mechanical behaviour around pore formed in solid oxide for SOFC. Comparison of the moduli shows that the effective modulus by homogenization method is closed to the measured data very well in the little porosity, the differences become large with the increasing of porosity. Moreover, the pattern of pore formation in the materials was explored using the technique, and discussion on the relationship between the homogeneous model and formation pattern of pore ware given .

Keywords: *simulation, homogeneous, SOFC*

C01

Integrated Fluid-Thermal-Structure Numerical Analysis for the Quenching of Metallic Components

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As metallic components with channel sections formed from annealed dual phase steels are quenched to form the desired strengthening microstructure, it was found that the amount of springback of the side walls of components depends on the direction of the sample in the quenching tank. In this paper, to reduce the distortion of the components and improve the heat treatment technology, the quenching was numerically simulated, which includes film boiling, nucleate boiling and convective cooling processes. CFD was used to model the multiphase flow and the heat transfer in the quenching tank to calculate the difference in heat transfer rate around the components and then combining with the thermal simulation and structure analysis of the components to study the effect of quenching rate on the distortion of the components. The heat transfer model was performed for different orientation of the components in the quenching furnace. A model was also established to calculate the residual stress fields of both forming and quenching. The austenite – martensite transformation was modeled based on the thermodynamic calculation and taken into account in the structure model. The predicted distortion profiles fit well to the measured. Coupling with structure modeling, the fluid-thermal-structure coupling modelling technology provides an insight into the deformation of metallic components in quenching oil and successfully be used to reduce the distortion of the components.

Keywords: *fluid-thermal-structure modeling, CFD, residual stress, phase transformation, forming, quenching, springback*

C02

Finite Element Modeling of Quenching Heat Treatment of AISI 4140 Steel with Phase Transformation

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Computer simulation of the quenching process has emerged as an economical and an important industrial tool to simulate the quench stress, distortion, microstructure and hardness. The objective of this work was to develop a finite element code to predict the temperature field and microstructure during quenching of AISI 4140 (a low alloy steel) and to test the applicability of the surface heat flux model proposed by Babu and Prasanna Kumar [1]. Though the finite element model developed in this work was used and tested for the simulation of quenching of AISI 4140 steel, the principles should be applicable to any practical heat treatment and welding processes of low alloy steels. The phase transformation model developed by Kirkaldy and Venugopalan [2] was used in this work for predicting the amount of phases transformed during quenching.

A quench probe with a diameter of 20 mm and length of 50 mm was machined from AISI 4140 steel. Deep holes with a diameter of 1.2 mm were drilled for a depth of 25 mm along the probe's axis and another one with its axis 2 mm offset from the cylindrical surface. K-Type thermocouples were fixed in these holes and temperature was recorded during quenching. The probe was heated to 850 °C, soaked for 10 minutes and quenched in still water. The micrographs taken at the mid plane consisted of full lath martensite at the surface and lath martensite with little feathery bainite at the core (Fig. 1).

The process was simulated in the finite element code for 25 seconds with 0.1 seconds as time step. The surface heat flux model proposed by Babu and Prasanna Kumar [1] was used as boundary condition for the simulation. The simulated time-temperature at the core and 2 mm below the probe's surface were compared with that of the experimentally measured values in Fig. 2. The simulation results of the microstructures were 87% martensite and 13% bainite at the core and 100% martensite at the surface. The simulated values of the temperature and microstructures were in good agreement with the experimentally measured values.

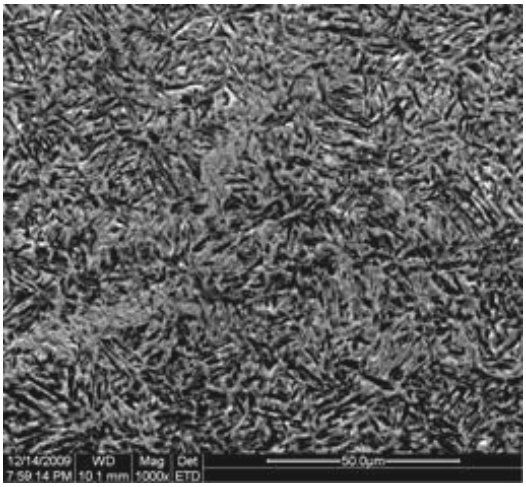

Fig. 1 Microstructure at the core

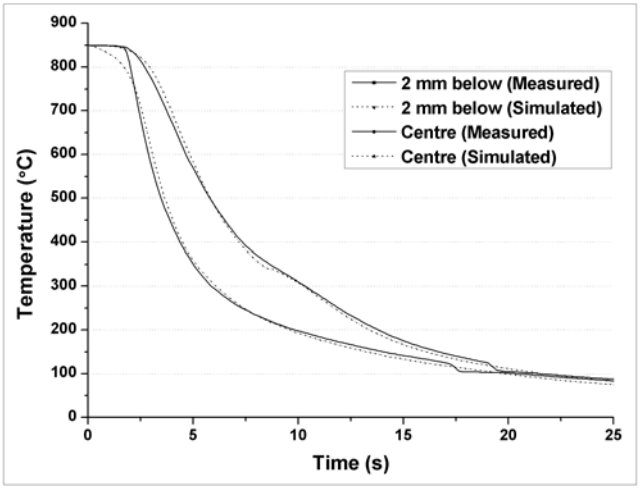

Fig. 2 Measured and Simulated time-temperature profile

Keywords: *modeling, quenching, heat transfer, phase transformation*

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C03

Mechanical Properties of Undercooled Aluminium Alloys and Their Implementation in Quenching Simulation

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Age hardening of aluminium alloys consists of solution annealing, quenching and aging. During quenching a supersaturated solid solution is formed, which is necessary for the following precipitation of strengthening particles. Further, during quenching thermal gradients occur in components, which can generate residual stresses and distortion. For heat treatment simulation, thermophysical properties, transformation behaviour and mechanical properties of materials are required depending on temperature and microstructure [1]. In the case of quenched aluminium alloys, mechanical properties mean mechanical properties of the undercooled alloys. The mechanical properties of these non-equilibrium microstructures are not available. Hot tensile tests of aluminium alloys can be performed at relevant temperatures, but their microstructures are near equilibrium and differ from the undercooled state. Therefore, compression tests of undercooled aluminium alloys like 6082 and 7020 have been performed in a quenching and deformation dilatometer. Samples have been solution annealed and quenched in the dilatometer with varying quenching rates (0.1 K/min to 1000 K/min) and varying quenching temperatures. Immediately after quenching, compression tests on quenching temperature have been performed in the dilatometer. The results have been correlated with continuous

time-temperature-precipitation-diagram of the aluminium alloys, which have recently been established by the authors using differential scanning calorimetry [2]. The mechanical properties like yield strength and strain hardening strongly depended on quenching rates and quenching temperatures. This could be explained by different concentrations of the supersaturated solid solutions as well as by different amounts of thermally activated dislocation movement. The stress-strain-curves could best be described by the Hockett-Sherby-model. This model and its parameters depending on quenching rates and quenching temperatures have been implemented in a quenching simulation by the finite element method. One important application is the quenching process of aluminium extrusion profiles directly after leaving the extrusion press [3].

Keywords: *aluminium alloys, age hardening, quenching, mechanical model, quenching simulation*

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C04

Vacuum Carburization B/D Schedule Design and Gas Quenching Response of AISI 9310 Steel Fatigue Sample

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Vacuum carburization process was applied to produce rotation bending fatigue test samples. The samples were machined from AISI 9310 steel bars. An acetylene/hydrogen mixture was used for the vacuum carburization process. The vacuum carburization schedules were designed using DANTE to through carburize the thin wall section of the fatigue sample. The samples were then gas quenched at 10 bar with nitrogen by Solar Atmosphere Inc. The microstructure and hardness, and distortion were checked to validate DANTE predictions. Some samples showed significant bow distortion after heat treatment. Further investigations on the sample shape response during quenching indicated that the unbalanced wall thickness is the main cause of the bow distortion.

C05

Influencing factors on cooling uniformity of large caliber seamless pipe for quenching

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Based on the current cooling method commonly used to cool outer surface by low pressure pipe jet and inner surface by high pressure axial jet, the numerical simulation by FEM software –ANSYS was performed to study temperature field of large caliber –seamless steel pipe for quenching. The factors considered are diameter of steel pipe, the rotation speed of steel pipe and the wetting angle of cooling medium –water. The numerical results reveal that pipe diameter is little influence on cooling uniformity. Radial cooling uniformity of steel pipe is preferable under the condition of the rotation speed of no less than 60 rpm and the wetting angle of around 270°.

Keywords: *seamless steel pipe, quenching, temperature field, cooling uniformity, numerical simulation*

C06

Modeling of Transformation Plasticity during Quenching Processes of Large Steel Forgings and Experimental Validation

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Dilatometric tests under uniaxial external loads are used to calculate transformation plasticity parameter. A continuous cooling dilatometric test is proposed to study bainitic transformation plasticity. The factors which have influence on values of transformation plasticity parameter are studied by using experimental results of several low alloy steels used to manufacture large steel forgings. It is found that values of transformation plasticity parameter can be fitted as a function of transformation temperature. Residual stresses of a hollow cylinder after water quenching were calculated and compared with measured results to validate the temperature-microstructure-stress coupled model. The evolution of temperature and internal stresses in a shaft connector during water-air alternative quenching processes were analyzed.

Keywords: *transformation plasticity, dilatometric test, quenching, internal stress*

C07

Prediction of properties of gas-quenched work pieces based on the modified hardenability test

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For steel grades of good and high hardenability, the Jominy test is not enough selective and sensitive. To establish hardenability for these steels a new hardenability testing method with the modified Jominy test specimen has been proposed. It is based on the high pressure gas end-quenching of cylindrical specimen with variations of kind of gas, pressure and its velocity to achieve more gradual decrease of cooling rates along the specimen and to make the hardenability test more selective with a broader range of lower cooling rates which are characteristic for gas quenching in vacuum furnaces [1]. The hardenability curves obtained by this new test were used for prediction of microstructure and hardness over cross section of gas-quenched cylinders made of steel grade EN 90MnCrV8 [2]. The following four models has been compared: Creusot-Loire calculations; Liscic-Filetin method with finding an equidistant points of Jominy curve and work piece, method with calculation cooling time from 800 to 500 °C at discrete points in work piece and finding their correspond hardness from hardenability curve; the phenomenological phase transformation model with kinetic equation of an Avrami type *[3-5]*. The simulated and experimental results of the hardness distribution and portions of microstructure phases of particular model have been compared and discussed.

Keywords: *hardenability, Jominy test, gas quenching, cooling time* $t_{8/5}$

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C08

Numerical simulation research on heat transfer of air mist spray cooling

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With the development of national economy, the requirement of die steel is increasing. At the same time, the comprehensive performance of die steel is required to improve. And some big steel mills have asked to apply on-line quenching in order to save energy consumption. Die steel usually contains high carbon and alloy elements. So in the quenching process, the cooling rate is reduced as far as possible to avoid deformation and cracking caused by excessive internal stress. The air mist spray cooling is the method that pressurized air makes water into mist spray. The range of cooling capacity is very wide from air cooling to water cooling. Therefore, the air mist spray cooling is a good way for die steel quenching. In this paper, the transfer heat characteristics between air mist spray and high-temperature plate are researched by heat-flow coupling method. When the discrete-phase volume fraction is less than 10-12%, the mixed convection heat transfer model is used. The effects of cooling parameters, such as air-water volume fraction, injection speed, gas-water velocity ratio, the distance of nozzle and plate, the temperature of the steel plate, on the heat transfer coefficient and the cooling uniformity are researched. The results of this study provide important reference value for the material controlled cooling equipment development and the actual production.

Keywords: *air mist spray cooling, quenching, numerical simulation, heat transfer characteristics*

C09

Computer Modeling and Validations of Steel Gear Heat Treatment Processes using Commercial Software DANTE®

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The heat treatment process of a gear made of carburized steel AISI 9310 is modeled using the commercial heat treatment simulation software DANTE. Both carburization and quenching processes affect the residual stress distribution and distortion of heat-treated parts, which are important to service quality and fatigue life. DANTE/VCARB is used to design the Boost/Diffuse schedule of a vacuum carburization process. Oil quenching is modeled following the vacuum carburization process. Thermal gradients and phase transformations are two main sources of distortion and residual stresses in quenched parts. The relation of the carbon distribution, thermal gradient, and phase transformations during quenching is studied through the gear modeling example. Because of geometry, the residual stress distribution after quenching is non-uniform along the gear surface. In general, the tooth fillet has higher residual compression than either the root or tooth face locations after traditional oil quenching of carburized gears. The predicted residual stresses from the oil quenching model are imported into a single tooth fatigue bending model. The gear stresses under bending load indicate the possible cracking locations during bending fatigue test. The importance of heat treatment residual stresses during gear design is pointed out, which is commonly ignored in the gear design and manufacturing industry.

Keywords: *vacuum carburization, distortion, residual stress, phase transformation.*

C10

Short-time tempering kinetics of quench hardened pearlitic steels

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In many industrial processes such as welding, and operating environments like railway wheel/rail contact, certain material volumes are exposed to very short temperature pulses that endure for times of the order of 1 s or shorter. When pearlitic steel is exposed to temperatures above the effective austenitisation temperature, martensite forms upon rapid cooling. In the current work tempering of a martensitic carbon steel was performed, with a laser heat source to create short time top-hat temperature pulses, and also with conventional salt bath experiments for longer tempering times. Temperatures were varied in the range of 500 to 700°C, and times between 0.05 to 3000 s. It was found that the martensitic test samples showed a very rapid initial softening upon tempering. During the first 0.1 second the hardness decrease was measured to 35-55% in the tested temperature range. Thereafter the additional hardness decrease was limited to ~10-15% of the original hardness, even after 30 min of tempering. Thus the use of time-temperature models for predicting tempering properties, that relies on constant or linear dependence of the activation energy cannot be extrapolated to very short time processes.

Keywords: *Tempering kinetics, Laser heat treatment, Martensitic steel, Hollomon-Jaffe time-temperature parameter*

C11

The Developments and Application of Computer Simulation Code on Induction Heat Treatment Process

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In the processes incorporating phase transformation, such as quenching, welding, casting and so on, the mechanical properties of manufactured material are necessary to be depended on coupled analysis of incorporating with temperature field, stresses fields and since the structural change due to phase transformation. The coupling analysis method based on the metallo-thermo-mechanical theory has been proposed by some studies [1]-[4]. However, simulation of some key processes have more complex physical phenomena, such as induction heating have to consider more physical behavior, for example, electric-magnetic filed an so on.

Induction heat treatment process has been developed as a key technology in manufacturing industry because of its superior characteristics. Induction heating reduces energy consumption, contributes to the protection of environment, and improves productivity. This paper describes the developments and application of computer simulation on induction heat treatment considered with coupling of temperature filed and magnetic field. In this paper, the developed simulation code COSMAP is introduced as a CAE software system for considering the design of induction heat treatment process covers all aspects of heat treatment simulation, from magnetic or electrical to thermal states, phase transformation, residual stresses including as well all metallurgical phenomena.

Keywords: *Induction Heating, Coupling analysis, metallo-thermo-mechanical theory, FEM*

C12

Heat transfer and process modeling in direct fired rotary kilns

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Rotary kilns are widely used in the chemical and metallurgical industry for thermal treatment of granular, fine grained and powdery materials. The process in a rotary kiln is influenced by a lot of parameters for example the rotational speed, inclination angle, diameter and length of the kiln. To optimize processes and to design rotary kilns the heat transfer has to described mathematically. The heat transfer in a rotary kiln is a complex phenomenon. In a direct heated rotary kiln heat is transferred from the flame or combustion gas to the free bed surface and the inner kiln wall, which consists of refractory material. A part of this heat is absorbed in the wall; the other part is reflected to the free solid bed surface. The absorbed fraction is partially conducted through the wall resulting afterwards in heat loss and partially transported to the covered bed due to the rotation of the kiln. Based on the heat transfer in the cross-section a theoretical process model is developed to calculate the axial temperature profiles of solid and gas in the kiln.

A pilot plant rotary kiln is used for ascertaining experimentally the heat transferred in the kiln. Therefore the axial temperature profiles of the solid bed, gas and wall are determined with thermocouples at different axial and radial positions along the kiln. The pilot plant rotary kiln with an inner diameter of 400 mm and a length of 5000 mm is directly heated by a natural gas burner. For experimental investigation the material and also the parameters rotational speed, mass flow and inclination angle would be varied. The analyzed materials are different in particle size, particle form, density and heat conductivity.

In present work the special measuring techniques will be explained in detail and the results for various materials and operational parameters will be shown. Furthermore the process model will be validated with the results of experimental measurements.

Keywords: *process modeling, heat transfer, temperature profile, pilot plant, rotary kiln*

C13

Thermodynamic Analytical Modeling of Gas Reactions to investigate the effect of Environmental Temperature and Humidity on Carbon Potential in Gas Carburizing Process

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In gas carburizing process, the amount of carbon potential of furnace is the most important specification of the process in term of achieving desired metallurgical properties.

In the present research, the gaseous reactions in an endothermic gas generator have been simulated and a thermodynamic analytical model been developed using MATLAB software. Subsequently, the carbon potential (resulting from burning methane in a gas generator) was calculated solving the equilibrium constant equations. Besides, The effect of important variables such as relative humidity and ambient temperature as well as air to fuel ratio in the endothermic gas generator, carburizing temperature and pressure inside the furnace have been investigated. Finally, results of the simulation have been compared with experimental results obtained from a gas carburizing furnace

Keywords: *Simulation, Gas Carburizing, Carbon potential, air to fuel ratio, relative humidity*

C14

First Principles Characterization of PhaseTi2AlN Prepared by Plasma Nitriding of Ti3 Al alloy

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Plasma nitriding of Ti-33Al alloy was successfully performed at 800°C for 2h in a mixed gas of 25% nitrogen and 75% hydrogen with different gas pressures. The surface phase constructions and nitrogen concentration in surface layer were analyzed using an X-ray Diffractometer (XRD) and Energy dispersive spectroscopy (EDS), respectively. The electronic structure and mechanical properties of the phase formed in the nitrided surface were also characterized by first principles calculations based on density functional theory (DFT).The experimental results show that the gas pressure has a strong influence on the proportion of Ti2AlN phase in the nitrided surface layer. The ratio of Ti2AlN phase can be increased greatly with the increase of the gas pressure from 133Pa to 400 Pa (Fig.1). The calculated results show that the covalent Ti-N bond is very strong while the Ti-Al bond is quite weak (Tab.1). The isotropic bulk modulus, shear modulus and Young's modulus are 156GPa, 120GPa and 286GPa, respectively. The ratio of bulk modulus to shear modulus is 1.30 (Tab.2).
This indicates that polycrystalline Ti2AlN possessing high Young's modulus and intrinsic brittleness.

Keywords: *Ti2AlN, First-principles calculations, plasma nitriding, mechanical properties*

c15

Thermal Flow Simulation and Visualization of PAG Quenchants in Cooling Evaluation Equipment with Twin Stir

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In order to evaluate cooling power of quenchants in quenching process, a new type of cooling evaluation equipment with twin stir was proposed. In optimization design of the stir tank, thermal flow and temperature filed under stirring with difference rectification structure are simulated. On the other hands, the formation and movement of bubbles in boiling film during quenching process was also investigated with high-speed video camera and PIV technology as means of visualization method. Cooling curves of surface temperature during quenching of steel cylinder are measured and the heat transfer coefficients between quenchant and steel are identified. The evaluation of the cooling ability of the coolant used for the quenching technology relates to the quality control in the machine part. As for this paper, the cooling capacity of the PAG quenchants(polymer solution) is evaluated. In addition, the heat transfer behavior in quenching process is clarified more than making of generation and the destruction of the thermal flow and destruction of the steam film by using the PIV method of visualization. Effect of mechanical stirring of quenchant on steam film and heat transfer is studied.

Keywords: *Thermal Flow, simulation, boiling film, heat transfer, Stirring.*

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C16

Modeling of Processes of Thermo-chemical Treatment of Metals: Traditions of Russian Scientific School

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The paper is devoted to 100th anniversary of the outstanding Russian scientist professor Yuriy Mikhailovich LAKHTIN – the founder of the world-famous scientific school of surface strengthening of metals and alloys. Lakhtin's scientific school is recognized for its contribution into research of processes of thermo-chemical treatment of metals and especially of nitriding. Today at the Department of Metal Science and Heat Treatment of MADI his followers continue the traditions of Lakhtin's scientific school. The development of technologies of surface engineering is based on complex modeling of physical processes realized by thermo-chemical treatment of metals. Thermodynamic models describe the interaction between metals and components of saturating atmosphere and predict phase composition of diffusion layer. Diffusion models of kinetics of saturation of metals allow to calculate the rate of growth of diffusion layer and regulation of its depth and structure. Structural models determine quantitative dependence between parameters of structure (grain size, dispersed particles, etc.) and mechanical properties. These models allow to estimate the level of strengthening by control of structural specifics of strengthened layer. On the basis of this complex of models new efficient technologies of surface strengthening are developed.

Keywords: *Lakhtin's scientific school, modeling of thermo-chemical treatment, nitriding, thermodynamic models, diffusion models, structural model*

C17

Numerical Analysis for Film Boiling Cooling Heat Transfer of Moving Hot Steel Plate

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The cooling of the steel strip in ROT (run out table) of the hot rolling process is very significant in the aspect of the fact that the ROT is the final process to control the mechanical properties of the final products. In general the products are cooled by the circular water jets which makes the comparatively thick residual water layer about 100~200 mm according to the supplied flow rate on the plate. The basic phenomenon which governs this cooling process is the boiling heat transfer. The boiling phenomenon is one of the most well-fixed heat transfer mechanism by the past a few decades research. However, almost all the results have been made by the experimental way. In this paper, we treat the boiling heat transfer on the moving hot plate with the fully numerical approach. The simulation was conducted only in the very high temperature region (over the Leidenfrost temperature) where the film boiling can keep steadily on the plate. The film (the steam layer) was regarded as the heat resistance whose capacity (actually the steam layer thickness) varied according to the plate surface temperature and the flow rate and temperature of the water jet. To predict the steam layer thickness which shows a very different spatially distribution on the plate, the continuity for the temperature and heat flux at the interface between the water layer and steam layer was managed to be satisfied by the iterative procedure for the effective thermal conductivity of the first node on the plate wall. The results for the cooling history of the plate, the heat flux as well as the temperature distribution in the direction of thickness which could not obtained by the experimental way are presented. The result for the temperature history is compared with the experimental results and showed a good agreement.

C18

Numerical Simulation for Thermal Process upon Reducing Gas Composition of Pre-Reduction Shaft Furnace

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Based on the principles of mass, momentum and heat transfers between two phases, the reducing gas and the iron ore solid, a two-dimensional mathematical model was established to study the thermal and reduction characteristics inside the pre-reduction shaft furnace of ironmaking process. The effects of the reducing gas composition upon internal thermal state of the furnace were also investigated by employing the model. The results showed that the optimal proportion of carbon monoxide to hydrogen in the reducing gas varied with its initial inlet temperature in order to yield high quality product, meanwhile replacing the reducing gas with an appropriate proportion of nitrogen with the same temperature could cut down the emission of carbon dioxide per ton product as well as obtain the product with the same quality.

Keywords: *mathematical model, thermal state, reducing gas composition, shaft furnace*

c19

Research on the quenching performance of 22MnB5 quenched in the steel die

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In order to research the effect of austenitizing temperature and holding time to the quenching performance of hot stamping boron steel 22MnB5, the experimental project is designed, and series of quenching process are done. The tensile strength and hardness of 22MnB5 samples are measured using the electronic tensile testing machine and Rockwell hardness tester, the effect of austenitizing temperature and holding time to the tensile strength and hardness of 22MnB5 is attained. The true strain-stress curves are computed and gained according to the results of experiment. The research results show that, 22MnB5 has a good quenching performance, the tensile strength and hardness of samples quenched using the steel die with cooling water system are similar to those of water quenching. The samples have higher tensile strength and HRC hardness when quenching at the austenitizing temperature 880℃-910℃. The tensile strength, hardness and ductility of quenched samples are better when holding for 5 min at the austenitizing temperature of 910℃.

Keywords: *Hot stamping boron steel; Quenching; Tensile strength; Handness*

C20

Geometric integral methods in simulation of thermal processes

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The paper discusses the simulation of applied heat engineering and thermal processing, in which for computer modeling of heat transfer used new approach based on integral equations of special type. Unknown functions in these integral equations are derived heat flows, so temperature is calculated by integrating the

found distributions with the initial and boundary conditions. In the obtained integral equations the upper and lower limits of integration depends on the geometric shape of the object, which leads to their name - the geometric integrals. Obtained integral description allows a natural way to make their discretization on the basis of average values of the unknown function at the specified intervals, and restore the function in endpoints.

In solving heat equations are often situations arise when the numerical scheme, based both on the finite difference method (FDM) and finite element method (FEM) leads to an oscillating behavior of the approximate solutions, which manifests itself either in the vicinity of discontinuities thermophysical properties or in areas with large temperature gradient. These problems arises, for example, in the numerical solutions of laser processing, as well as in processes in which there are phase transitions of first or second kind (process of heat treatment of ware). Additionally, the finite element methods as well as FDM are difficult to estimate the accuracy of the results.

The main advantage of the proposed approach is the opportunity not only to avoid the "nonphysical" oscillation in the numerical solution of the heat, but also to evaluate the accuracy of the obtained approximation with the discrepancy in the system of integral equations. An additional feature of the geometric integrals method is the fact that it largely allows the use of parallel computing for solving three-dimensional tasks in geometrically complex areas.

There are the results of simulation of the unsteady temperature fields in variety of composite materials and modeling the process of surface hardening of rolls. Shown physical adequacy found distributions of temperature and heat flow, as well as consistency of results with different grid partitions.

Keywords: *integral equations, numerical methods, heat flows, accuracy, software*

c21

Timed Quenching Process for Large-scale AISI 4140 Steel Shaft

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The mechanical properties of AISI 4140 steel shaft with a diameter larger than 200 mm are difficult to satisfy the requirements due to insufficient cooling ability of oil quenching, and cracking occurs easily in water quenching because of too rapid cooling. A new technology named Alternately Timed Quenching (ATQ), using water and air in turn as the quenching media instead of oil or polymer aqueous solution, is applied to quench the large-scale AISI 4140 steel shaft. In the present work, two ATQ processes are determined with the aid of computer simulation first and the corresponding physical experiments are carried out consequently. The results show that the proposed technology can significantly reduce the surface cracking tendency and improve the mechanical properties in practical production of such large-scale shaft forgings.

Keywords: *Computer simulation; quenching; cracking; mechanical properties*

c22

Kinetics of Austenite Grain Growth in Medium-carbon Nb- bearing Steel

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To confirm a reasonable heating system, austenite grain growth behavior of a Nb microalloyed medium carbon steel has been experimentally studied at various austenitizing temperature and for different holding

time. It is indicated that the austenite grains grow with the increases of austenitizing temperature and holding time. Austenite grains grow rapidly and abnormal austenite grain growth were observed, when austenitizing temperature is above 1100℃. When austenitinzing temperature is lower than 1100℃, austenite grain size and growth rate are small. The activation energy of grain growth in the tested steel is 397.7KJ/mol. The heating technology of the tested steel should be controlled in 1 hour at about 1100℃ for insuring no obvious coarse grains in microstructures. The relationships of austenite average grain size with soaking temperature and time of tested steel by mathematical calculation are obtained, and calculated austenite average grain size is in agreement with the measured size for different holding time.

Keywords: *microalloyed steel, grain growth, modelling*

c23

Development and Application of Computer Simulation Code COSMAP on Induction Heat Treatment Process

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Induction heating reduces energy consumption, contributes to the protection of environment, and improves productivity. This paper describes the developments and application of computer simulation on induction heat treatment considered with coupling of temperature filed and magnetic field. In this paper, the developed simulation code COSMAP is introduced as a CAE software for considering the design of induction heat treatment process covers all aspects of heat treatment simulation, from magnetic or electrical to thermal states, phase transformation, residual stresses including as well all metallurgical phenomena.

Keywords: *Induction Heating, Coupling analysis, metallo-thermo-mechanical theory, FEM*

D01

Numerical analysis of unconventional forging process of hollowed shaft from Ti-6Al-4V alloy

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This paper presents theoretical analysis of unconventional forging process of hollowed shaft from Ti-6Al-4V alloy in a three-slide forging press. This method in comparison with other metal forming methods, allow for obtaining of hollowed products. The designed process was verified theoretically by means of numerical simulations based on finite element method with the assumption of 3D state of strain. The following factors were considered in the analysis: material flow kinematics, strain distribution, temperature distribution and force of process. On the basis of results, it was stated that the application of designed technology allowed for obtaining of a product of assumed quality. A comparison was made between material consumption in analyzed process and material consumption in typical metal forming methods, also in used at present technology of shaft manufacturing by machining only. It was stated that the application of forging in the three-slide forging press will allow for a considerable decrease of manufacturing costs due to material savings and decrease of labor consumption of operations at finishing.

Keywords: *Hollowed shaft, Die forging, Three-slide forging press, Finite element method*

D02

The analysis of the cross-wedge rolling process of toothed shafts made from 2618 aluminum alloy

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The paper presents the results of a thermo-mechanical analysis of rolling two stepped shafts. One of the shafts has a toothed step with skew teeth, while the other has a worm winding in the shape of a trapezoidal screw. The shape of the rolling tools resembles that of the tools used in the Roto-Flo rolling method; yet unlike in Roto-Flo, the shafts are hot rolled and no centres are used to stabilize the position of the workpiece during the forming process. For the calculations made with use of the DEFORM-3D process simulation system it has been assumed that the rolled shafts are made from 2618 aluminium alloy. As a result of the calculations made, it has been found that toothed stepped shafts can be formed in one pass by means of the cross rolling process. Additionally, the temperature and strain distribution in the rolled product have been determined as well as some data concerning the forces which are necessary for the rolling process have been obtained.

Keywords: *cross rolling, toothed shafts, 2618 aluminium alloy, FEM*

D03

FEM temperature simulation of accelerated cooling on Run-out Table during hot rolling

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Control of temperature during accelerated cooling is essential for achieving desired mechanical and metallurgical properties of steel. Due to the high speed of a strip and complex circumstance, it is very hard to set up a cooling model with high accuracy for temperature predication, especially for inner temperature distribution of cooled strip.

In this study, finite element method (FEM) simulations with a model validated using actual plant data have been conducted. To achieve an accurate temperature field, the effects of various factors are taken into account, including different velocity and position of coolant water flow, cooling patterns and various rolling parameters. In addition, temperature risen model after cooling is also set up, and modeling of temperature profile during water cooling are focused on. Comparisons between the predicted and actual measured results are used to illustrate the validity of the FEM model, and it shows there is a good agreement between predicted temperature and measured temperature.

Keywords: *Mechanical properties, Temperature control, FEM simulation, Accelerated cooling, Hot rolling.*

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D04

Fractal studies on primary phase morphology of the TA15 titanium alloy after hot compressive deformation

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The goal of this study was to establish relationships between the hot compression deformation behaviors and fractal dimension D of the primary phase morphology of TA15 titanium alloy using the analytical methods of metallurgical microscope and transmission electron microscope coupled with box-counting dimension method. Hot compression deformation behaviors varied with decreasing fractal dimension D owing to the change of microstructure caused by the different technological parameters of hot compressive deformation. The results indicate that TA15 alloy shows dynamic recrystallization characteristics at deformation temperature lower than 850℃ while the fractal dimension D exhibits a moderate decreasing trend with the temperature increasing, shows dynamic recovery characteristics at deformation temperature higher than 850℃ while the fractal dimension D reduces rapidly with the temperature increasing. The results show that

D displays non-linear relationship with percentage content of primary phase and with aspect ratio of primary phase.

Keywords: *compression deformation behaviors, fractal dimension D, TA15 titanium alloy, box-counting dimension*

D05

Simulation experiment on friction coefficients during warm deep drawing of magnesium alloy sheet

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In sheet metal forming, friction condition between sheet metal and mold is a very important problem for it influences the formability and the variation of stress, strain and thickness of sheet metal, and so on. Simulation experiments had been done to measure friction coefficients online at punch and die rounded corners under different process parameters during warm deep forming of magnesium alloy sheet. The results made it clear: temperature shows the greatest effect on friction coefficients, the blank holding force(BHF) of their effect secondly, and no significant effect of lubricant on the friction coefficients. The friction coefficients at die rounded corner are larger than those at punch rounded corner. The dynamic changed friction coefficients models with temperature and blank holding force were fitted by the experimental data respectively, and they were added into simulation software through further development by user subroutine VFRIC using FORTRAN language to improve the accuracy of the numerical simulation.

Keywords: *magnesium alloy sheet; warm deep drawing; friction coefficient; simulation experiment*

D06

Study on Temperature Evolution and Metal Flow of 6005A Aluminum Alloy during Indirect Hot Extrusion

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In the present paper, a numerical model has been build up for the prediction of temperature evolution and metal flow for the extrusion of 6005A aluminium alloy. The results were compared with the experimental data for model validation. Both simulation and experiment show a good agreement with each other. The influence of the extrusion parameters on the profile temperature and metal flow were studied according to the real industrialized extrusion. It was found that the profile temperature increases with the ram speed as well as the peak load of the total press force. However, a too slow extrusion process would cause increasing of the total force at the end of the extrusion because of heat dissipation to the environment. In addition the dead metal zone at the top of the billet was shrunk during the extrusion process. The ram speed would have little influence on the distribution and evolution of dead metal zone. It also showed that once the extrusion went into steady stage, the strain rate of metal flow would keep a stable situation relatively.

Keywords: *indirect extrusion, Finite element modeling (FEM), aluminium alloys, metal flow, temperature*

D07

Research of Al-Mg-Si alloy hot-rolled multi-stage recrystallization by experiment and simulation

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Al-Mg-Si alloy samples were compressed discontinuously on the Gleeble-1500 thermal-mechanical machine to test multi-pass hot-rolled deformation, and their deformation forces were measured. After the compression, the microstructures and were analyzed by observation of OM and TEM, and the micro-hardness of deformed samples was tested. Based on the above experiment results, a Monte Carlo simulation model was established, and used to simulate the Al-Mg-Si alloy hot-rolling dynamic recrystallization and static recrystallization. The results show that: the Al-Mg-Si alloy would undergo significant dynamic recrystallization and static recrystallization during hot-rolling; the recrystallization softening effect is understood through the deformation force curves and the hardness curves; the Monte Carlo model effectively simulates dynamic recrystallization and static recrystallization organizations, and emulates the evolution process of recrystallization.

Keywords: *Aluminum alloy, recrystallization, Monte Carlo, simulation*

D08

Recrystallization Behavior of a Ti-microalloyed Complex Phase Steel During Hot Compression

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Double-hit isothermal deformation and multipass continuous cooling hot compression tests were taken to study the recrystallization behavior of a 0.11% (mass) Ti-microalloyed complex phase steel (CP steel). The influence of different deforming temperature and different holding times on microstructure transformation was investigated. The results showed that a pronounced austenite grain refinement after appropriate recrystallization process has been detected. The grain size decreases continuously from 176um to 20um after four passes compression. It has been verified that non-crystallization temperature (Tnr) of the experimental steel is about 950℃。The grain was elongated at deformation temperature lower than Tnr. Based on the stress-strain curves and the static recystallization behaviour at isothermal deformation, a kinetic equation was estabilished to predict the recrystallization fraction of Ti-microalloyed steel during nonisothermal continuous hot deformation. The calculated results of equation have been compared to metallographic measurements. There is a good correlation between the experimental and calculated results.

Keywords: *Ti-microalloyed complex phase steel, recrystallizaion, nonisothermal hot deformation*

D09

Influence of soaking temperature on microstructure of multi-pass compression deformation for low carbon steels

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The influence of soaking temperature on microstructure of high temperature multi-pass compression deformation for two low carbon steels (0.032C-0.25Mn, 0.165C-0.38Mn) is studied on the thermal-mechanical simulator in order to rationalize the hot-rolling schedule of low-carbon steel and to promote the low-temperature heating technology. The results show that the microstructures of 0.032C-0.25Mn steel are almost not affected by reducing soaking temperature, but the acicular ferrite formed in 0.165C-0.38Mn steel when the soaking temperature reduced from 1200℃ to 1170℃, due to its smaller initial austenite grain size according to recrystallization kinetics theory.

Keywords: *Soaking temperature; multi-pass compression deformation; Low-carbon steel*

d10

The Study of Warm Surface Rolling of Steel 45 Groove Axle

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Warm surface rolling is a process working between room temperature and below re-crystallization temperature. After warm surface rolling of steel grade 45 groove axle was carried out, its fatigue lifespan was measured by endurance bending test. The influence of surface rolling reduction to the axle fatigue life period was experimentally studied at different surface temperatures. The research results show the fatigue life of axles could be significantly improved by warm surface rolling process. The optimum rolling reductions for maximum fatigue strength at different warm rolling temperatures were explored. The microstructures of the axles were analyzed. The surface strength improved by refining grain size is calculated by Hall-Petch model. These research achievements would be also valuable to the similar researches.

Keywords: *surface hardening, warm surface rolling, physical simulation, fatigue lifespan*

D11

String-like Atomic Motion in Metallic Glass under Deformation

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The development and use of advance and sustainable materials via controllable experimental strategies such as heat treatments and solidification requires basic understanding of atomic-level mechanisms.

In metallic glasses, plasticity is believed to be intimately associated with the cooperative atomic motions in string- or chain-like form. Albeit of both theoretical and application importance, many aspects of the corresponding dynamics remain so far unclear.

Using molecular dynamics (MD) simulations, we aimed to characterize atomic motions in Cu-Zr metallic glasses under deformation. String-like cooperative motions at temperatures far below the glass transition are observed. To capture the essential dynamics, the mean length and distributions of the strings are measured, which are found to depend strongly on both strain and temperature. Our MD observations provide useful hints to understand the mechanical behaviors of metallic glass, esp. the origin of shear band formation.

Keywords: *String-like atomic motion, Metallic glass, Plastic deformation, Molecular dynamics*

D12

The Forging Penetration Efficiency of Steel H13 Stepped Shaft Radial Forging with GFM Forging Machine

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The numerical thermal mechanical simulation of radial forging process of steel H13 stepped shaft with GFM forging machine was carried out by three dimensional finite element method DEFORM 3D. According to effective plastic strain, mean stress and mean plastic strain distribution of the radial forging process, the forging penetration efficiency (FPE) was studied throughout. The results show that: effective plastic strain in the center of the forging area is never be zero; The mean stress in the center of the workpiece is proposed to describe hydrostatic pressure in this paper. There is compressive strain layer beneath the surface of the workpiece, while there is tensile strain layer in the center of workpiece. These studied results could be a valuable reference for designing the similar forging operations.

Keywords: *radial forging, forging penetration efficiency (FPE), stepped shaft, finite element*

D13

Thermal-mechanical Coupling Simulation and Springback Control in Hot Forming Process of Fan Blade

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As an aeration equipment, fan blade is one of the most important mechanical components. The fan blade in this case has a 3D anomalistic surface. By using a drawing process there are many difficulties such as billet’s location, material waste, etc. Especially, drawing process needs large forming force, and workpiece will rebound seriously after drawing. That’s the mainly reason why a hot forming process is used.

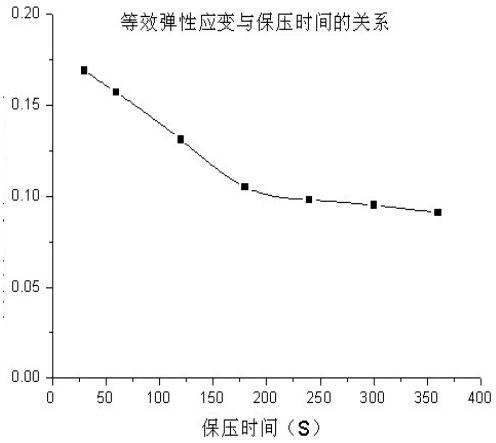
According to the shape features of fan blade, hot forming process means high temperature and large deformation. Many factors, such as heat transferring on billet-die interface and heat generated by deformation and friction simultaneously, make temperature field of billet continually changed. The change of temperature field will affect deformation behavior, mechanical capacity, and microstructure of blade furthermore. Therefore, it is important to using thermal-mechanical coupling simulation in DEFORM-3D platform to research on hot forming process of fan blade for optimization of forming technology. A brief introduction of the project and its main results are as follows:

The key technical problems of 3D thermal-mechanical coupling rigid-viscolastic FEM simulation of fan blade forming process are studied systematically. A 3D thermal-mechanical coupling FEM simulation model corresponding to reality is set up for the hot forming process of the fan blade. By using the DEFORM-3D, the orderliness of the fan blade hot forming process is revealed, and an important function of temperature in

forming process is indicated. The distribution of spring back, warping and the stress-strain in the forming laws of hot forming process is obtained.

Based on the result of simulation, billet’s spring back after forming and cooling can be predicted. The final spring back is beyond the error range. Then a new process specification which appends a pressure maintaining process is made. There are 7 projects of different time made for the pressure maintaining, and the results of simulations in DEFORM-3D are as follows:

Time of pressure maintaining(s)	Equivalent elastic strain max(mm)
30	0.169
60	0.151
120	0.131
180	0.105
240	0.098
300	0.095



360	0.091

According to the numerical value of equivalent elastic strain max in the table above, the orderliness of fan blade pressure maintaining process is revealed. Equivalent elastic strain max - time of pressure maintaining curve is as follow:

When billet was kept 60s of pressure maintaining after hot forming, the workpiece’s spring back could be acceptable.

Finally, a scheme of trial-manufacture is designed according to the simulation conditions. After the trial-manufacture, the measurement of fan blade’s spring back is permitted by the error range, and is in accordance with the simulation result. It indicates that numerical simulation could play a guiding role in experiment, but should be validated by experimente.

The experiences of simulation and trial-manufacturing of fan blade provide a practical, efficient, economical and reliable forming process for the related industries which produce this kind of blade parts.

Keywords: *hot forming of fan blade, thermal-mechanical, spring back discipline, validity check of experimental manufacture*

D14

Numerical simulation for effects of friction on quality of low alloy steel forgings

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In metal forming processes, friction plays a significant role in determining the life of the tool, the formability of the work material and the quality of the finished product such as, surface finish, internal structure, and product life. Friction can increase the inhomogeneity of deformation, leading to defects in the finished products. Friction can also be used beneficially to manipulate the material flow to achieve the desired end product with a minimum effort [1-4].

In order to study the workability and effects of friction on dynamic recrystallization in deformed low alloy steel, the compressive deformation behavior of 42CrMo steel was investigated at the temperatures from 850 to 1150℃ and strain rates from 0.01 to 50 s^{-1} on Gleeble-1500 thermo-simulation machine. Based on experimental results, the dynamic recrystallization mathematica1 models of 42CrMo steel were derived. Then, the thermo- mechanica1 coupled finite element model was developed to investigate the effects of friction on dynamic recrystallization in a deformed 42CrMo steel during hot upsetting were investigated by integrating the thermo-mechanica1 coupled finite element method with the derived microstructural evolution models. The results show that the distributions of strain/stress in the deformed block are inhomogeneous, and the degree of the deformation inhomogeneity changes with the frictions between work-piece and dies. The distribution of dynamic recrystallization volume fraction and dynamic recrystallization grain size, which change with the frictions, are also inhomogeneous in the deformed work-piece. Also, the friction significantly affects the broadening coefficient of the forgings.

Keywords: *forging, friction, low alloy steel, microstructural evolution*

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d15

Simulation on Rolling Force and Temperature Field of Plate Steel during Hot Rolling

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Rolling force and temperature field are important technological parameters in hot rolling process of plate steel. Most researchers use ANSYS/LS-DYNA and MSC. Marc to simulate hot rolling process, however, software DEFORM-3D is not used widely in this field. Therefore, in this study, the commercially available FE analysis software DEFORM-3D is used to simulate the distribution of rolling force, stress-effective, strain-effective, temperature field during the hot rolling process of plate steel with the size of 230*1400*3060mm. Both the simulated rolling force and temperature of the multi-pass are compared with the measured results, meanwhile the effect of relative factors on the simulated accuracy during hot rolling has been discussed. The result shows that the simulated values by the finite element method are approximate to

the measured values in plate steel. So the simulation can provide an important reference and optimization to make rolling process and parameters in steel factory.

Keywords: *Simulation , Hot Rolling Force and Temperature Field, Plate Steel, Software DEFORM-3D*

D16

3D Finite Element Simulation of Rod and Wire Continuous Rolling

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This paper discusses the application of several techniques involved in the development of the 3D finite element (FE) models of rod and wire continuous rolling process. The FE models are implemented into the FE-program MSC.Marc and used to investigate the thermal and mechanical behavior of billet during the rolling process. All nonlinear equations included in the models are solved by static and dynamic procedures respectively. Data transfer technique is proposed to keep the continuity of simulation results. And the computational time of static procedure is significantly reduced by using a rigid pushing body. In all models, constant time step method and auto time step method are respectively used to define time step for the solution of equations. Simulation results of the models with different time step methods are compared. And comparison between calculated values and measured ones of the temperature at the surface of billet shows the validity of the FE models.

Keywords: *rod and wire rolling, 3D FE simulation, data transfer, auto time step*

d17

Dynamic Recrystallization Model and Simulation Analysis of SPCC steel Hot Rolling

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In this paper, thermal simulation equipment Gleeble-1500, right SPCC steel at different deformation under the true stress - strain curves were determined in conjunction with the microstructure observation, identified SPCC steel dynamic recrystallization of a mathematical model study and analysis of deformation parameters for dynamic recrystallization grain size effects. Through the finite element software DEFORM right SPCC steel thermal compression process simulation. Analysis of the different deformation conditions on the grain size effects. Finally, the simulation results well coincide with the experimental results.

Keywords: *SPCC steel; dynamic recrystallization; mathematical model; finite element simulation*

D18

Numerical simulation analysis in cooling temperature field and bending deformation after rolling of 100-meter rail

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Different parts of the cross section have different cooling speed in rail cooling process , resulted in different parts of the cross-section cause different shrinkage deform capacity and different times of producing phase swelling, makes repeated bending phenomenon happens to the direction of rail head and rail foot during cooling, rail have obvious bending deformation and residual stress after cooling, the more the phenomenon is

obvious the more the rail is longer. If the rail adopt advance to the reverse bend to the rail foot before cooling, then the rail is flat after a period of time in cooling. The article base on fundamental principle of the heat transfer analysis、 thermo- elastic-plastic analysis、contact analysis and finite element analysis theory, established 3-d transient nonlinear finite element analysis model about U75V 100- meter rail by using large non-linear finite element analysis software ABAQUS. Analyzed the section of the different positions of temperature variation in the cooling process if the 100-meter straight rail in natural cooling, simulation results show that deflection changing with time can mainly divided into four stages in the cooling process:(1) in the early cooling 100s inside, rail deformation slightly to track rail foot of bending trend; (2) in the 150s ~400s period of time, the whole rail bends toward the rail head;(3) in the 400s~650s period of time, no deformation have occurred in rail, for equal to inflation;(4) in the 650s~900s period of time, the whole rail bends toward the rail foot,(5) in the 800s~10000s period of time, the whole rail bends toward the rail head, but the deformation rate go to smooth, in the end of cold, When the time is 10000s reach to final bending deformation, the maximum is 1.88 m, thus eventually puts forward the reasonable scheme by applied for 100-meter rail recurvation and cooling conditions.

Keywords: *100-meter rail, temperature field , bending deformation, numerical simulation*

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D19

Research and Application of Pre-bent automatic control Models of 100 meters rail

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Repeated bending occurs toward the direction of rail head and rail base during the cooling which can lead to significant bending deformation and residual stress after cooling, the longer the rail, the more obvious this phenomenon is. In addition to cooling function, a kind of cooling bed with a pre-bending process will be used in order to solve this problem on 100 meters rail. The synchronous movements on this cooling bed can be realized by the automatic control system after establishing the mathematical model of bending deformation after rolling. The rail is reversely bent toward the rail base before cooling according to the pre-bending control of the pre-bending curve and is straight after cooling which can realize the control of the residual stress after pre-bending and straightening. The straightening residual stress significantly reduced after the pre-bending.

Keywords: *100 meters rail, pre-bend, control model*

D20

Simulation of Large Forging Flat-anvils Stretching Process and its Optimization

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Distribution of strain during stretching process is related to tool width ratio and reduction. It is believed by experience that distribution of strain is fairly reasonable and defects can be closed effectively with the value of tool width ratio 0.5-0.8 and of reduction 20-25%. Infected by friction and hard deformation area near two terminal , distribution of compress strain near the axis is difficult to be continuous and uniform, and defects lied in the hard deformation area is difficult to be healed. With a certain values of feed, fairly uniform deformation in the central axis will be obtained and internal defects can be closed during the stretching process. Research has shown that the specific values of feed is usually determined by experiments and manufacture experience, and that there has never been quantitative calculation , which brings some deviation inevitably .The quality of large forgings can’ t be assured scientifically and quantitatively.

In this paper, a new mathematic method of optimizing stretching process of large forgings is proposed. Distributions of effective strain within forged ingots is described by a Gauss function, which was obtained from simulating of the flat-anvils stretching process. Successive stretching is expressed by superimposing Gauss functions. Optimized stretching process, with both homogeneous and certain strain in the center of forgings, is presented by derivation of this function. The relationship between effective strain and the values of feed was obtained during successive stretching with rotation angle 90° and a feed displacement of 1/2 anvil width. The optimization result is verified by finite element simulation. Optimized values of feed obtained through this method can ensure both uniformity and forging penetration. It provides mathematic model and theoretic basis of optimizing large forgings stretching process.

Keywords: *large forgings, flat-anvils stretching, numerical simulation, optimization*

D21

A study of FCC metal tension behavior by crystal plasticity finite element method

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The crystal plasticity finite element method (CP-FEM) has been adopted to study the slip system activation, the number and magnitude of active slip system, the rotation character and the macro mechanics response of FCC single crystal metal during the uniaxial tension. The five typical crystalline orientation (including four type of typical FCC texture orientation: Goss orientation, copper orientation, S orientation and brass texture) has been introduced and its effect to plastic deform character has been studied and compared. The work indicate that different angle relationship between crystalline and loading direction will affect slipping character and macro-mechanical response: the S crystalline orient(60°, 32°, 65°)has the least number of active slip system (just only 3); brass texture (35°, 45°, 0°) have the smallest magnitude of crystalline lattice rotation; the brass texture orientation (35°, 45°, 0°) has the highest yield stress value.

Keywords: *FCC metal, tension behavior, crystal plasticity, CP-FEM, slips system*

D22

Simulation of the tube forming process in Mannesmann mill

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In this paper, the finite element method (FEM) is used for simulation of the tube piercing process in Mannesmann mill. The numerical model is described with taking into consideration thermal phenomena in metal during forming. The simulated results visualize dynamic distributions of mean stresses, temperature, velocity and shear stresses, especially inside the workpiece. On the basis of the basic parameters, the phenomenon in the piercing process is analyzed. The model was verified by comparing the values of calculated force parameters of the piercing process and those measured in laboratory conditions. Finally, the future plans are presented.

Keywords: *FEM analysis; Simulation; Tube piercing process*

D23

A Novel Monte Carlo Potts Model in Metal Rcrystallization Simulation

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Some new advices are proposed for Monte Carlo Potts model of re-crystallization annealing simulation, including an additional recovery process, a new stored energy distribution, a more advanced nucleation model and a conversion probability of site orientation. Then a novel Monte Carlo Potts model is established absorbing the above improvements, and used to isothermal annealing simulation of 1060 pure aluminum cold-rolled sheet. For contrast, a re-crystallization annealing experiment of 1060 pure aluminum is carried out at the same time. The results show that the 1060 aluminum alloy in the annealing experiment produces obvious re-crystallization, and the grain morphology after re-crystallization are similar to isometric. The new model can effectively simulate the non-homogeneous nucleation process and the microstructure evolution of 1060 industrial pure aluminum in annealing, and the simulated re-crystallization kinetics curve is similar to the theoretical curve, and the Avrami exponent n_{av} coincides with the experimental result but is lower than the theoretical value of 2. As the model isn't involved with texture, the isometric grains simulated are not completely consistent with the experimental results, and because the model does not consider the preferential growth orientation, grain size in the simulation organization is less than the experimental result.

Keywords: *re-crystallization; Monte Carlo; simulation*

D24

Study on Bending Conditions of Plate in Coil Box

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In a coil box between the roughing and finishing stands on a hot strip mill, a problem has been encountered that the entry region of the plate touches the bending rolls and deforms. As a result, the defective coil occurs. The condition of plate bending, which forms a new deformation feature in coiling, is analyzed. In this paper, the authors focus on the research of the effects of coiling parameters, such as the thickness of plate, roll speed and feeding speed of plate in coil box, on specific plate bending. A finite element method is developed to simulate this coiling process. Based on numerical simulation, the effects of the coiling parameters on the mechanics and deformation of the bending plate are obtained. Numerical simulation tests have verified the validity of the developed model.

Keywords: *Profile, Plate Bending, Finite Element Method, Coil box, Hot Strip Mill*

D25

The Microstructure prediction of magnesium alloy AZ31D during hot extrusion

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A set of constitutive equations was proposed for hot extrusion of magnesium alloy, which can describe the single peak dynamic recrystallization. The parameters in the equations were obtained from the compression test. An inverse extrusion process was performed for magnesium alloys AZ31D at high temperature. In order to predict the microstructure evolution during the hot extrusion, a user-defined subroutine describing the constitutive equation were implanted into the commercial software, DEFORM2D, to simulation the hot extrusion process. The predicted microstructure distribution shows a good agreement with the experiments.

Keywords: *AZ31 magnesium alloy; Dynamic recrystallization; Constitutive equation; Microstructure evolution*

D26

The application of numerical simulation technology to the forming process of large scale tee

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Deformation behavior of the X80 at high-temperature was studied. The stress-strain curves at different temperatures were measured by means of GLEEBLE-1500 and GLEEBLE-3500 thermal simulator. Key forming parameters of the large scale tee, the round-corner of branch pipe and the temperature of billet, were analyzed using numerical simulation method. The reasonable range of these two parameters was determined. Acceptable products were made based on the simulation result.

Keywords: *large scale tee, X80, forming process , numerical simulation*

d27

Orientation evolution during equal channel angular pressing of aluminum single crystal

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Initial crystallographic orientation plays a very important role in plastic deformation because it dominates many aspects of material behavior, such as strength, dislocation structures, grain refinement, and plastic anisotropy. In the present study, a crystal plasticity finite element method model has been developed to understand the influence of initial orientation on texture evolution of aluminum single crystal oriented (-1 -1 2) [-8 18 5], subjected to equal-channel angular pressing using a die having a channel angle of Φ=90° and an outer arc of curvature Ψ=30° for one pass at room temperature. Textures predicted by the developed model are in good agreement with the experimental observations. The simulation results have shown a counter-clockwise rotation around the transverse direction, a clockwise rotation around extrusion direction and a clockwise rotation around insert direction after ECAP deformation.

Keywords: *equal channel angular pressing (ECAP), crystal plasticity FEM, aluminum, single crystal*

d28

Study on Formability about ME20M Magnesium Alloy Sheet

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Warm forming of magnesium alloy sheet has attracted more and more attention in recent years. Mechanics tension test has been made in this paper in order to study the constitutive relationship of ME20M magnesium alloy sheet at different temperatures and strain rates. And a constitutive relationship which includes a softening factor has been put forward. Warm deep drawing experiment and numerical simulation on ME20M magnesium alloy sheet have been made in which the attention was focused on the forming temperature. The results showed that the limit deep drawing height of ME20M magnesium alloy sheet can be dramatically improved as the temperature goes up, especially when the temperature was over about 250℃. Simultaneity, it is feasible and effective to add a material model into numerical simulation software through by user subroutine.

Keywords: *ME20M magnesium alloy, formability, constitutive relationship, further development*

d29

Simulation of Hot Deformation of Spray Formed 7XXX Alloy with High Zn Content

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The hot deformation behavior of a 7XXX series Al alloy (Al-10.5Zn-2.0Mg-1.5Cu) processed by spray forming (SF) was investigated by isothermal compression tests in the temperature range 340℃-460℃ and strain rate range 0.001s-1-1s-1 using Gleeble-1500 heat physical simulation system. The results reveal that the true stress－strain curves exhibit a peak value at a critical strain, after which the flow stresses slightly decrease until high strains, showing a dynamic flow softening behavior. Furthermore, the flow stress is controlled by the strain rate and deformation temperature, where decreasing temperature or increasing strain rate causes an enhancement in the peak stress level. It was also concluded that a Zener-Hollomon parameter Z in the hyperbolic-sine equation can be used to describe such stress level. By means of multiple linear regression, α, n, A and hot activation energy Q were determined as 0.017MPa-1, 5.329, 3.164×109s-1 and 146.569 kJmol－1, respectively. The constitutive relationship for the studied alloy was established which offers a basic model for plastic forming simulation.

Keywords: *hot deformation behavior; constitutive relationship; spray forming; 7XXX alloy; Zener-Hollomon parameter*

d30

Study on Computer Simulation and Superplastic Extrusion of AZ31B Seamless Tube

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Used the Gleeble-1500D thermal-simulator, the superplasticity of magnesium alloy AZ31B, was explored and the relationship between flow stress and true strain were achieved at different temperature. Then the digital model of deformation structure was established using Pro/Engineer software. The computer simulation of superplastic extrusion with different extrusion velocity was processed by DEFORM-3D software. From the simulation results, the distributing of equivalent strain and the metal flow characteristies was analyzed also. The forming temperature and extrusion velocity was optimized as 360℃, 2～6mm/min respectively. The experiments of superplastic extrusion for AZ31B seamless tubes were carried out to test the results of computer simulation. It was found that the magnesium alloy seamless tubes could be manufactured with good appearance and inner quality. That is to say, the model and computer simulation for superplastic extrusion of magnesium alloy tube was reliable and effective.

Keywords: *magnesium alloy, seamless tube; computer simulation, superplastic extrusion*

d31

Study on The Finite Element Numerical Simulation of Automobile Beam Stamping Forming

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This paper is concerned with the effect of design parameters on the stamping process of automobile beam. The considered parameters in this paper are the Friction coefficient, the Die fillet radius and the blank holding force, which greatly affect the metal flow during stamping. Based on the finite element numerical simulation, the stamping shaped process of the automobile beam is numerical simulated with various parameters by dint of DYNAFORM software. According to the simulation results, the forming limit diagram(FLD) and the wall thickness distribution of cloud on the stamping processes are analyzed ,the reasons and control methods of wrinkling and rupture are also pointed out ,and then the optimal parameter combination of the automobile beam is obtained by orthogonal experiments.

Keywords: *stamping forming, numerical simulation, orthogonal experiments, parameter optimization*

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d32

Computer Simulation of the Continuous Annealing Recrystallization for Cold Rolled Strip Steel in Galvanizing Line

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The continuous heating transformation program was developed to investigate the influence of technological parameters of continuous annealing on recrystalization for cold rolled strip in galvanizing line. This program can be used for the calculation of the strip steel continuous annealing temperature field, determination of the start and end time of recrystallization in continuous heating process, and procurement of the continuous heating transformation diagram. The continuous annealing temperature field was simulated with finite difference method. Based on the Scheil superposition principle, the continuous heating transformation curve during cold rolled strip continuous annealing was obtained by using time temperature transformation (TTT) curve which was measured experimentally. The developed program has been used by some manufacturers. The strip steel speed of the line was increased by more than 10%, and the output was raised 3 million tons per annum.

Keywords: *cold rolled strip steel, continuous annealing, recrystallization, continuous heating transformation, time temperature transformation*

d33

Numerical simulation of U-channel forming process of quenchable steel at elevated temperature

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The application of high-strength quenchable steel can significantly reduce the weight of automotive body structure and maintain the safety requirement. Hot stamping is a new type process in which the blank is formed at austenite temperature and quenched in the cold closed die. In this paper the hot stamping process of the quenchable steel is investigated in experimental and numerical method with a common u-channel part. The experiment presents the thermo mechanical properties of the steel. A material model and a geometrical model were set up under the hot stamping conditions. With these models, the u-channel forming process was simulated with ABAQUS software. The result presents the stress-strain field and the temperature field. With these the Wall thinning at the key point and the forming limited of the material were analysis. The result also shows the influence of the temperature on punch press.

Keywords: *hot stamping, numerical simulation, high strength steels, u-channel forming*

D34

Design of flash structure for forging die based on intelligent optimization algorithms

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The novel flash structure of forging-die: resistance wall, can greatly improve material utilization, but the forming load would greatly increase and the die life would be shorted if the parameters of resistance wall were designed improperly. In this study, the screening test for the parameters of the resistance wall structure were carried out and the variables which have an obvious affect on forming load are decided. According to these variables, the numerical simulations are carried outs based on experiment design and the approximation model for resistance wall is established by the Kriging interpolation method. The particle swarm algorithm and genetic algorithm is used respectively to optimize the model. The results show that the optimal values of two algorithms have high consistency. Finally, the optimal parameters of the resistance wall structure are obtained.

Keywords: *forging-die , screening design , particle swarm algorithm , genetic algorithm*

D35

Research on Pores Deformation Welding Condition for Manufacturing of Heavy Forgings

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Crushing and diffusion welding are two critical healing stages of interior void defects of heavy forgings. The healing result depends on many complex factors during forging process, such as stress state, temperature, deformation degree and type of material, while the void diffusion welding condition is still not well known at the present time. The present work is concerned with the deformation welding condition of the closed void interface in heavy ingot during hot forging process. A void crushing experiment was carried out to recognize the microstructure of the closed void interface. According to the healing mechanism at high temperature, a new physical simulation model was setup to study the deformation welding process of the closed void interface based on the theory of atom diffusion and the interface contact mechanics prototype. From the experimental results, the influence of deformation degree, forming temperature and holding time on welding quality was discussed, and then the deformation welding condition of closed void interface was presented. The proposed condition will help to improve forging technology and product quality.

Keywords: *large forgings, interior void defects, physical simulation, deformation welding condition*

d36

FEM Study of The Tensile Behavior of Annealed ULC-BH Steels

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ULC-BH(ultra low carbon bake hardening) steels were annealed in a salt bath with a temperature range from 740℃ to 830℃ followed by water quenching. Then, tensile tests were carried out to determine the mechanical properties of specimens treated by different annealing processes. Results indicated that the strength of the test steels were almost the same, while the elongation rates changed largely due to the nonuniformity of specimens dimensions and the heterogeneous distribution of precipitates. To overcome these shortcomings, ANSYS/LS-DYNA was employed to simulate the tensile behavior of the ULC-BH steels by setting the experimental strength data as the initial parameters. The effects of annealing temperatures on mechanical properties were simulated and the best mechanical properties and their corresponding parameters were obtained. These best mechanical properties with optimum parameters were validated by experiments.

Keywords: *ANSYS/LS-DYNA, simulation, mechanical properties, ULC-BH steels, annealing processes*

D37

Numerical analysis of the effect of material properties on the deformability of near hemispherical shell

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The deformability of near hemispherical shell is mainly determined by material properties and shell structure. In this paper, the effects of hardening exponent, yield strength and Young's modulus on the deformability

are investigated by finite element method (FEM). The largest eccentric angle during the deformation process (βm) and thickness reduction after the deformation (Δtm) are introduced to estimate the deformability quantitatively according to the deformation characteristics of near hemispherical shell. Furthermore, the orthogonal experiment design is used to arrange the simulation. The results indicate that the hardening exponent is the most influential parameter followed by Young's modulus and yield strength. The shell is in good deformability when the hardening exponent and Young's modulus are in the range of 0.1-0.125 and 70-90Gpa respectively.

Keywords: *Near hemispherical shell, Deformability , Orthogonal experiment design, FEM, Material properties*

D38

First-principles prediction of ductility in β-type Ti-Mo binary alloys

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Recent studies suggest that the ratio of shear modulus (G) to bulk modulus (B) and Poisson's ratio (ν) are good indicators of ductility. Using the method of supercell and the first-principles pseudopotential plane-wave method, the G/B and ν of the β-type Ti-Mo binary alloys with Mo content ranging from 6.25 at.% to 37.5 at.% were calculated. The results show that the ductility of β-type Ti-Mo binary alloys first increases with increasing Mo content and reaches the maximum when Mo content is about 25 at.%, and then reduces with more increasing Mo content. The charge density difference calculations suggest that the Mo content dependence of the ductility can be ascribed to the change of bonding characteristics between Ti and Mo atoms in the [111] direction.

Keywords: *Ti-Mo alloys, first-principles, ductility, charge density difference*

d39

Asymmetric deformation of near hemispherical diaphragm under uniform surface load: Simulation and Experimental

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The asymmetric deformation and eccentricity problems of near hemispherical diaphragm under the uniform surface load are quantitative characterized firstly in present work. The analysis is based on a three-dimension finite element analysis (FEA) model which established according to elastic-plasticity and large displacement nonlinear finite element method. Besides, the deformation experiments are taken to validate the reliability of FEA model which shows that the simulation results are in good agreement with the experimental results. Then, three angle parameters, β, θ, γ are introduced and expressed to characterize the asymmetric deformation and eccentricity quantitatively. According to the angle parameters, the inversion process of uniform thickness diaphragm and varying thickness diaphragm are calculated respectively. The inversion process of varying thickness diaphragm is much steadier than uniform thickness diaphragm. The present results show that the asymmetric deformation process can be characterized by (β, θ, γ) curve exactly, the degrees of eccentricity can be indicated by βw and the eccentricity position can be characterized by (βw, θw, γw).

Keywords: *Deformation, Hemispherical Diaphragm, Finite Element Method, Eccentricity*

D40

Microstructural modeling of dynamic recrystallization in Nb microalloyed steels

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Prediction of microstructural evolution in thermo-mechanical processing is of important to obtain good final properties for HSLA steels. This work presents a physical based microstructure model to describe the microstructural evolution in controlled rolling. Dislocation density, recovery, recrystallization and precipitation have been coupled as several interactional submodels in the model. The dynamic recrystallization (DRX) behavior of Nb microalloyed steels has been investigated. The recrystallization is described as a nucleation-grain growth process, and critical dislocation density has been used to estimate the occurrence of dynamic recrystallization. Moreover, the state of element Nb in hot rolling has great impact on the DRX. When the Nb element in solution, the increase of Nb content in solution will raise the apparent activation energy in deformation of matrix, improve the flow stress, thereby enhancing the critical strain need to be dynamic recrystallization occurred. NbCN precipitates significantly delays recrystallization by precipitate-pinning mechanism.

To characterize the dynamic recrystallization behavior of Nb microalloyed steels, a series of multi-stage compression tests were carried out after complete austenitization. From modulating the parameters of the model, the prediction of microstructural evolution at various hot rolling conditions agree well with the experimental results. It can effectively predict the relation among the time, the dynamic recrystallization rate and the recrystallization grain size under different deformation conditions of hot rolling.

Keywords: *Nb microalloyed steels, dynamic recrystallization, microstructural modeling*

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D41

Hot-Rolling Bonded Multilayered Composite Steels and the Varied Tensile Deformation Behavior

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Multilayered metal composites consisting of alternating metals or alloys have been well investigated to obtain the superior mechanical properties different from those in any of the constituent materials, such as fracture toughness, fatigue behavior, impact behavior, wear, corrosion and even deformability. Among those researches, there are a lot of reports focusing on the crack propagation behavior in brittle/ductile multilayered composites. However, the tensile behavior and its mechanisms of the composite with the aim to improve the deformability by the composite structure design are left for further investigation. The Layer-Integrated Steel and Metals (LISM) research project sponsored by Japan government started from 2006 and aimed to

fabricate steel sheets with high strength (>1200MPa) and superior elongation (>20%), through the composite design of martensite steels and ductile steel layers.

In the present work, two kinds of hot-rolling bonded multilayered composites consisting of austenitic stainless steel/ bainite (martensite) steel are focused. The effects of hot-rolled microstructure and the annealed microstructure on the tensile behavior are discussed. It is found that the large-reduction hot-rolling may cause a specific microstructure different from the normal microstructure of the constituent layers, and annealing treatment is key important to obtain the ideal strength-elongation balance. On the other hand, the tensile deformation microstructure of the hot-rolling bonded and annealed 15 layer composite steel is systematically investigated in order to find the reason for the enhanced plasticity of the brittle layer in the composite. The varied deformation mode and the gradient microstructure features formed in the deformed brittle layer are considered to cause the larger plasticity of the brittle layer in the multilayered composite.

Keywords: *multilayered composite, hot-rolling bonding, tensile behavior, EBSD analysis*

d42

Numerical Simulation of Expanding Process for Hollow Billet during Extrusion Steel Tube

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Expanding process of hollow billet is an important part of steel tube extrusion process. In this paper, finite element method is adopted to simulate the effect of deformation parameters and die on the deformation stability during expanding process. The result shows that expansion elongation, expanding cone angle and lubrication condition is the main factor affecting on stability during expanding for hollow billet. Increasing of expansion elongation and expanding cone angle, and bad lubrication conditions will cause deterioration of stability during expanding process, while increasing the length of expansion residue. The deformable temperature has no notable effect to the deformation stability.
Keyword: *expanding, deformation stability, expansion elongation, expanding cone angle*

E01

Computer Simulation of microstructure and distortion during quenching and tempering process of medium carbon steel

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Microstructure, stress, distortion, and hardness occurring during quenching and tempering of a medium carbon steel have been predicted using a commercial finite element software, ABAQUS with user subroutines including phase transformation kinetics, heat transfer, and mechanical properties. The fraction of each phase was obtained from the relationship between the measured dilatational strains and theoretical atomic volume of each phase during quenching and tempering. Thermal and mechanical properties were experimentally measured as functions of temperature and each phase. The residual stresses were measured by X-ray diffraction tests. The predicted results, such as phase fractions, distortion, residual stress, and temperature, were compared with the measured counterparts.

E02

Dimensional Analysis of Distortion during Through Hardening of Cylindrical Steel Workpieces

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The former investigations on the dimensional analysis of distortion during through hardening of cylindrical workpieces illustrated the significance of Biot number with a discussion of general problems and workarounds [1-2]. In another study [3], the authors conducted a sensitivity analysis of material properties for quenching, which revealed martensite start temperature (Ms), Koistinen-Marburger constant (Ω), transformation strain (ε tr) as the most sensitive parameters.

In this study, as suggested in the outlook of [2] and [3], the effect of dimensionless numbers with sensitive material parameters was demonstrated as a function of Biot number by computer simulations. The results indicate that investigated dimensionless numbers govern both the position and the shape of the dimensionless number vs. Biot number curves.

Keywords: *distortion, through hardening, dimensional analysis, dimensionless numbers, SAE 52100*

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E03

Generation of Compressive Residual Stresses by High-Speed Water Quenching

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According to literature, rapid water quenching can create compressive residual stresses near the surface and hereby a significant increase of the fatigue-limit results. This method is called "Intensive Quenching". In the present paper, the results from a research project will be presented, which was initiated by the technical committee "Quenching" of the AWT to deal critically with this issue.

The main goal in the project was, to acquire the ability to generalize the basically mechanism of the creation of residual stresses near the surface. Therefore, a lot of experiments where made with a newly developed quenching facility and a series of simulations were accomplished. It could be verified, that for the bearing steel SAE 52100 (100Cr6) the BIOT – Number could be used to characterize the surface residual stresses after a through hardening process. This dimensionless number is defined as

$$Bi = \frac{\alpha \widetilde{L}}{\lambda}$$

with the heat transfer coefficient α, the thermal conductivity λ and the volume to surface ratio $\widetilde{L}$ as the characteristic length. So it summarizes parameters from process, material and geometry.

As a central result, it was shown that by increasing this parameter above a critical value, residual compressive stresses near the surface could be obtained for through-hardened parts. Based on this results, a specimen for an endurance test was developed and an increase of the fatigue limit could also be achieved. .

Keywords: *High-speed water cooling, SAE 52100, 100Cr6, through hardening, roller bearings, simulation, compressive residual stresses, increase of the fatigue limit*

E04

Using Simulation for Heat Treat Process Design: Matching the Quenching Process with Steel Grade and Product Geometry

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The performance of steel parts is heavily dependent on the heat treat process applied. The alloy content of the steel establishes the steel hardenability. The severity of the quench establishes the local temperature history throughout the body of the part. In combination, the steel hardenability and the quenching process determine the final microstructure, mechanical properties, residual stress state, and the performance of the part.

The residual stress state, especially the surface stress state is a significant factor in affecting fatigue life of the part. The steel hardenability and quenching practice can be adjusted to enhance residual surface compression and improve the fatigue life of a component. Computer simulation of the heat treat process that includes calculation of the metallurgical phase transformations during the heating and cooling processes offers a method for scientifically designing the heat treat process and selecting the steel alloy to optimize the performance of a particular product. In this paper, the DANTE® heat treat simulation software will be used to demonstrate this design methodology for a spur gear.

Keywords: *quantitative characterization, heat treat simulation, phase transformation kinetics, dilatometry, residual stress*

E05

Comparison between High Pressure Hydrogen Quenching and Oil Quenching of Steel Parts Considering Load Effect

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Recently high pressure gas quenching (HPGQ) is getting more and more popular for its advantages such as environmental friendliness, low distortion, etc, compared to oil and water quenching. In HPGQ process, heat transfer coefficient (HTC) usually varies from part surface to surface because of the intense variation of gas velocity around the part. In addition, the work load also affects the HTC in both magnitude and distribution. This article studies the variation of HTC distribution of steel parts in a work load during gas quenching and oil quenching and compares the cooling severities of high pressure gas quenching and oil quenching. The distortions of the steel parts in gas quenching and oil quenching are also numerically studied and compared. The uniformity of cooling severity in a work load during gas quenching is also studied.

Keywords: *high pressure gas quenching, oil quenching, heat transfer coefficient, distribution, distortion, work load*

E06

Effect of Alloy on the Distortion of Oil Quenched Automotive Pinion Gears

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In a previous work [1,2], the distortion of 8620 carburized automotive pinions was determined via CFD, FEA and actual measurements. In an effort to reduce costs, and to reduce the distortion further, other common carburizing alloys were examined for the effect of alloy on distortion. The methodology and results of this work are shown

Keywords: *Finite Element, distortion, residual stresses, carburizing, quenching, transformation.*

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E07

Modelling of distortion during cooling and machining of aluminium engine blocks with cast-in cast iron liners

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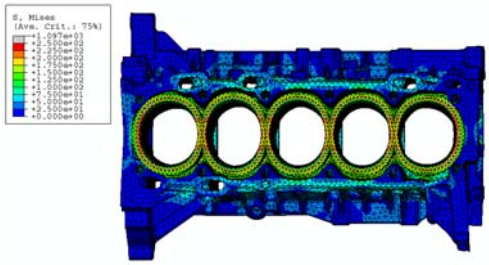
The paper discusses aspects of the process modelling of Out-Of-Roundness (OOR) of cylinders in five-cylinder engine blocks made of aluminium with cast-in grey iron liners. The main focus lies on the cooling/shrinkage modelling of the pressure-cast engine block and the build-up of high residual stresses. The stresses mainly arise from the difference in thermal expansion between the two materials and as stresses build up, the temperature and strain dependent relaxation of the aluminium becomes important. The modelling also concerns the redistribution of residual stresses during boring of the cylinders, leading to continuously developing OOR and increased machining costs.

The flow stress curves for the aluminium alloy were determined at temperatures from – 60° C to 350° C at strain rates of 10-5 s-1, 10-3 s-1 and 10-1 s-1. The specimens were taken from the material volumes around the cylinders of real engine blocks, specially fabricated without cast iron inlays to avoid pre-straining. The testing showed that the material exhibits pure elastoplastic behaviour up to 200° C but becomes increasingly strain rate dependent at higher temperatures. To capture this behaviour, two different viscoplastic models were calibrated and compared - one Perzyna model and one model available in ABAQUS called the "two-layer viscoplasticity model". As it turned out the latter model was the better for this application and it was therefore used for the OOR simulations.

To validate the modelling, OOR measurements have been done on blocks in between boring operations in the cylinders (i.e. the blocks were taken off the production line, measured and reinserted until the next boring operation was done). The OOR after cooling of the cylinders is correctly predicted at the top of the block (see figure below), but some deviation exists in the lower part of the cylinders.



Cyl. 2 – 4	x-direction	y-direction
Computed	rnom – 0.2 mm	rnom + 0.2 mm
Measured	rnom – 0.2 mm	rnom + 0.15 mm

Computed vs measured out of roundness close to the top plane of the engine block. Distortion magnified 20x

Keywords: *viscoplasticity, experiments, model calibration, residual stresses, distortion, engine block*

E08

Effects of Inhomogeneous Distributions of Distortion Potential on Out of Roundness of Rings

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Causes for distortion phenomena are inhomogeneities or asymmetries of the distributions of mass, alloying elements, microstructure, and residual stresses. These collectivity of causes generate a distortion potential of the work piece. In a previously published paper [1] the influence of inhomogeneous distribution of Martensite start temperature (Ms) was investigated by means of simulations with the commercial FE program SYSWELD® .

One of the most important results of that paper was an equation which describes the formation of out of roundness values of bearing rings. A parabolic dependency on 1/N (N represents the mode of harmonic analysis) was found. This result is consistent to many experimental investigations concerning the shape changes of rings due to hardening processes [2] and therefore probably true for many different distortion potentials within bearing rings.

For this reason this problem was investigated in a more general way. By an analysis of the bending radius it was found that the parabolic dependency of the out of roundness on the mode of harmonic analysis is a general characteristic of thin walled rings and therefore true not only for the distribution of Ms but for other kinds of distortion potentials too.

It will be shown, that local distributions of distortion potentials of bearing rings can be divided in two general parts. If the distortion potential varies only in circumferential direction the out of roundness depends linearly on the mean radius of the bearings rings, whereas a distortion potential which varies additionally in radial direction the resulting distortion depends to the power of two on the mean radius.

Keywords: *distortion engineering, bearing rings, harmonic analysis*

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E09

Prediction and Measurement of Residual stress for 6061 Aluminum Alloy during T6 Heat Treatment

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Aluminum alloys are used to many industries such as aircraft, automotive, and appliances due to their high strength to weight ratio and corrosion resistance. Aluminum-magnesium-silicon (Al-Mg-Si) denoted as 6XXX series alloys are medium strength heat treatable alloys. Mg and Si are the major solutes and they

increase the strength of the alloy by solute and precipitate hardening during T6 heat treatment involving quenching and ageing process. But, the thermal gradients of quenching and ageing can be large enough to produce high levels of residual stress[1].

These residual stresses can have a detrimental effect on the component leading to warping or cracking during quenching process, dimensional instability during machining process, the reduced fatigue life and the increased susceptibility to stress corrosion cracking[2]. Therefore, it is very important to reduce and relief the residual stress during heat treatment. In order to relief the residual stress, it needs the measurement and prediction of residual stress according to heat treatment conditions.

The purpose of this study predicts the residual stress of Al6061 during T6 heat treatment according to conditions of solid solution and ageing time. The Al6061-T6 heat treatment procedure is shown in Fig. 1 and specimens of heat treatment experiment are given in Fig. 2. This study conducts the prediction and measurement of residual stress during T6 heat treatment. The prediction of residual is analyzed by elasto-plastic nonlinear FE-simulation. In order to consider the solute and precipitate hardening, FE-simulation is used in DEORM-3D V6.0 with USER SUBROUTINE. Also, residual stress is measured by X-ray diffraction (XRD) which is conducted to confirm the result of FE-simulation. Residual stress predicted by FE-simulation is in good agreement of with measured residual stress. Finally, this study can predict the residual stress of Al6061-T6 heat treatment with solute and precipitate hardening.

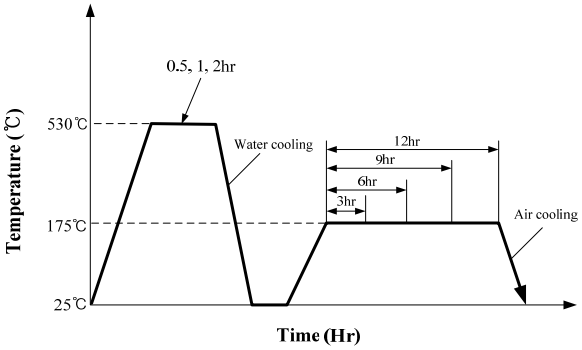

Fig. 1 T6 heat treatment diagram of Al6061.

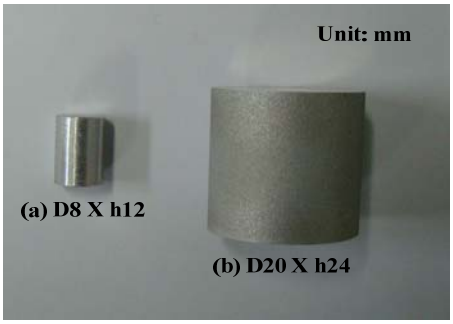

Fig. 2 Specimen of T6 Heat treatment.

Keywords: *Residual stress, Solid solution, Precipitate hardening, X-ray diffraction(XRD), FE-simulation*

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E10

Microstructure Evolution and Residual Stresses in Coke Drum Repair Welds

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Delayed coking is a thermal cracking process used in petroleum refineries to upgrade and convert petroleum residuum into liquid and gas products, leaving behind a solid concentrated carbon material called petroleum coke. The thermal cracking process takes place in coke drums. One whole coking cycle may last 24 to 48 hours. Coke drums fail at different lives due to fatigue. Typical life spans for a through wall cracking to occur range from 3,000 to 5,000 cycles or around 5 years in operation.

Cracked coke drums can be repair welded. Post weld heat treatment of repaired coke drums, however, is cost prohibitive. Weld repair of coke drums without post weld heat treatment is cost-effective but technically challenging. Controlled deposition weld repair have been demonstrated to meet the code requirement of coke drum repair without post weld heat treatment.

Advanced finite element models are used in this study to analyze the heat transfer, microstructure evolution, properties and residual stress development in controlled deposition repair welds. The test plates are 1.25 inch thick, which includes 1.125 inch steel substrate and 0.125 in clad. The substrate material is made of 1.25Cr-0.5Mo steel per ASTM A387 Grade 11. The clad is made of ferritic stainless steel per AISI 410S.

Predicted microstructural results are found in good agreement with experimental test results. It is found that over 80% grain refinement can be achieved with the given weld procedure. Hardness in weld heat affected zone can be reduced to below 248 HV per code requirement in most regions. There are discrete regions with high HAZ hardness.

E11

Numerical Modeling of the Stress-and-Strain State of the Surface Layer of Steel at High-Frequency Pulse Treating

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Determination of the residual stresses induced in steel during its treating by powerful high-frequency pulses demands usage of the complex models considering the electromagnetic, thermal, metallurgical and mechanical phenomena [1, 2]. In the given study the numerical two-dimensional model is considered in which on the basis of evolution of a temperature field induced in a cross-section of carbon hypo-eutectoid (steel 45) and hyper-eutectoid (steel U10) workpiece during treating by single electromagnetic pulse, the kinetics of phase transformations and evolution of thermoelastoplasticity state of material are calculated.

The model includes the Maxwell’s and heat conduction equations with the boundary conditions that accord to acting of a narrow stretched source of electromagnetic field on a semi-infinite carbon steel body [3]. Kinetics of austenitic transformation was determined by carbon isoconcentrate 0.02 wt.% position within grain that been obtained by diffusion problem solving. Final radial carbon distributions within grain of steel allow thereinafter taking into account the dependencies of martensitic transfer critical points on local carbon content. System of equations was approximated by implicit finite difference schemes and solved with alternating directions and under-relaxation methods on uniform mesh. Calculations were performed for frequency 440 kHz, specific energy flux 15 kW/cm2, pulse duration 30 ms and heat-affected zone width 2 mm.

Keywords: *carbon steel, pulse induction treating, phase transformations, stress analysis, simulatio*

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E12

Computer Simulation of Microscopic Stress Distribution in Complex Microstructure using a Phase Field Model

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Stress distributions in complex microstructures such as dendritic, cellular, and columnar structures are simulated using a phase field model. To enable this kind of simulation, fundamental equations are formulated considering the coupling effects among phase, temperature and stress/strain [1]. The model is also extended for a binary alloy system, where the coupling among phase, stress/strain and chemical composition is taken into account. An elasto-plastic constitutive equation is applied for the stress analysis, and stress evolution and residual stress distribution are simulated [2,3]. Complex microstructures are generated depending on the thermal conditions as well as nuclei set. For example, a dendritic structure is formed during solidification in a super-cooled environment from a single nucleus, and a cellular structure is obtained for directional solidification from multiple nuclei on a wall boundary. The stress distribution is then generated due to both the volumetric change by the phase transformation and thermal contraction in the solidified region. When the solidification completes in the whole region, the phase becomes homogeneous, while the residual stress distribution is observed. Large stress is generated especially when grain boundaries are generated, and the specific distribution is observed depending on the morphology of the microstructures. In the simulations for the binary alloy system, the effect of stress on the solid-liquid interface is also investigated. Considering the stress dependency of the phase transformation, the instability is affected by the stress distribution, and the different morphology is obtained. Additionally, as a typical phenomena in the directional solidification process, liquid droplets and grooves are generated in the microstructure, and large stress concentrations are observed around them. Finally, a simulation for a mixed structure of columnar and equiaxial crystals, which is typical in casting process, is demonstrated, and the relationship between microstructure and resultant stress is discussed totally.

Keywords: *Phase field model, Solidification, Residual stress, Microstructure, Computer simulation*

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E13

Finite Element Modeling of Hydrostatic Stresses Distribution in Copper Dual-Damascene Interconnects

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Hydrostatic stresses of copper interconnects were calculated with the dual-damascene models in the present work. Numerical work using commercial finite element package ANSYS, and analytical work were performed to examine the effects of different low-k dielectrics, barrier layer and aspect ratio of via on hydrostatic stresses distribution in the copper interconnects. The results of calculation indicate that the

hydrostatic stresses are highly non-uniform throughout the copper interconnects and the highest tensile hydrostatic stress exists on the top interface of lower level interconnect near the via. Both the high coefficient thermal expansion and low elastic modulus of the low-k dielectrics and barrier layer can decrease the highest hydrostatic stress on the top interface, which can improve the reliability of the copper interconnect. Moreover, hydrostatic stress is strongly dependent upon different low-k dielectrics, barrier materials and aspect ratio of via in the copper interconnects.

Keywords: *copper dual-damascene interconnects, hydrostatic stress, finite element modeling*

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E14

The research on controlling the pre-bending deformation before straightening and the residual stresses after straightening of 100-meter rail

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The repeated bending of rail is caused by different shrinkage or swelling capacity of different parts of rail with irregular cross-section during cooling after hot rolling. The straightness and residual stresses of the rail after straightening are affected by the bending deformation during cooling before straightening. By analyzing the heat boundary condition in the cooling process, the bend deformation is simulated by using the 3-D transient non-liner finite element method. The effect of the pre-bending deformation before straightening on the residual stresses after straightening is researched by controlling the bending deformation before straightening and the straightening deformation, drawing a conclusion that the residual stresses are affected by different chord heights at the same straightening rule, and the calculated results have a good accordance with the measured values on site.

Keywords: *100-meter rail, pre-bending deformation before straightening, straightening deformation, residual stress*

E15

Distortion Measurement of Martensitic Stainless Mold Steels using Vacuum Heat Treatment

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Two martensitic stainless steels were vacuum heat treated using different quenching and tempering processes. Some of the steel specimens were plasma nitrided at 420℃. The distortion analysis, microstructure, X-ray

diffraction and hardness of the treated specimens were conducted. The distortion was measured using a Mitutoyo micro-meter at 20℃. The results showed that the hardness of SUS420J2 and STAVAX ESR reached 57.5 and 57.2 HRC when austenitized at 1050°C for 25 minutes, followed by N2 gas quenching. From X-ray diffraction analysis, the phases of the quenched and tempered specimens consisted of martensite. The hardness profiles shows a strong hardening effect by the plasma nitriding and the hardness value of the nitrided layers were higher than 1000 HV0.05 due to the precipitation of a fine and homogeneous γ'-Fe4N, ε-Fe2–3N and CrN nitrides in the α'N matrix. The distortion variation in specimens austenitized at 1020℃, gas quenched and tempered at 480℃, was lower than those austenitized at 1050℃ for both SUS 420 J2 and STAVAX ESR specimens. The dimensional change in the longitudinal and transversal direction of the DCPN treated SUS 420 J2 and STAVAX ESR specimens was lower, both below 0.01%, compared with quench and temper treatment specimens.

Keywords: *Martensitic stainless steel, Vacuum heat treatment, Gas quench, Distortion*

E16

Simulation of Asymmetrical Quench Distortion of Long Thin Steel Parts

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This report focused on quench simulation of asymmetrical distortion (bending and warping) of steel parts or tools. Bending or warping in quenching is often observed for long thin steel parts. Asymmetrical shape of a steel part increases the degree of asymmetrical distortion. In the other hand, nonuniform heat transfer coefficient (HTC) on the steel part also increases it. The sharp edges of steel parts results in the premature collapse of vapor blanket on the quenched part, and as the result, increase the nonuniformity of HTC and the asymmetrical distortion.

Quench simulation result showed that the bending or warping of long thin steel parts is mainly resulted from longitudinal plastic strain of supercooled austenite in high temperature cooling phase, and the strain is controlled by the thermal stress in quenching. The result also shows that the thermal stress largely depends on nonuniformity of cooling of steel part. These analyses clarified the mechanism of bending and warping distortion during quenching of long thin parts.

The simulation accuracy of the quench distortion was studied by the comparison between the simulation result and the experimental result. It is not easy to estimate the nonuniform HTC on the surface of quenched steel part like a long thin blade. However, the consideration of the effect of the shape of steel part on HTC in quenching is often important to improve the simulation accuracy. In order to estimate the nonuniform HTC, the combination between lumped heat capacity method and inverse method was employed. We confirmed that the edge effect, i.e., the effect of shape edge on HTC, is important for simulation accuracy.

Keywords: *quenching, simulation, steel part, distortion, heat transfer coefficient*

F01

Measurement of Heat Transfer Coefficients during Downward Solidification of Commercially Pure Zn and ZA8 Alloy

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Casting solidification modelers require heat transfer coefficients for two reasons. One is to model solidification to identify the possible location of shrinkage defects. In this case the measured heat transfer coefficients under one gravity environment are quite suitable for applying to a situation where the solid casting surface is in (imperfect) contact with the mould wall. In the second case, models of heat transfer during mould filling are being used to try to predict casting misruns, where the cast alloy freezes before filling the mould cavity, and to predict the heat lost by the alloy during the filling process and hence the correct temperature distribution with which to begin the subsequent solidification modeling. In this case, the approach described above probably does not give accurate measurements of the heat transfer coefficient owing to the effect of fluid flow. By carrying out these measurements in a microgravity environment, fluid flow process caused by pouring or by natural convection, which would reduce the accuracy of a terrestrial measurement, would be avoided. However, duplicate experiments should be carried out in normal gravity conditions to assess the actual effect of natural environment on the accuracy of the measured heat transfer coefficients in each case. The methods adopted by the various researchers for the assessment of interface heat transfer were mostly based on the inverse heat-conduction problem (IHCP).

The present research work is aimed at the study of the effect of chill material, chill surface condition and superheat of casting on the casting / chill interfacial heat transfer during solidification of commercially pure zinc and ZA8 alloy. Copper, hot die steel, stainless steel and aluminum were selected as chill materials. Chills were instrumented with thermocouples to measure temperatures near the mold/metal interface. An inverse heat conduction model is employed to estimate the transient heat flux from the measured temperature field and thermo-physical properties of the chill material. Experiments were carried out at two different casting pouring temperatures and with and without coating on the chill surface. Metallographic studies were carried out to assess the effect of casting/chill contact heat transfer on the fineness of the microstructure near the interface.

The estimated heat flux curve shows a maximum shortly after pouring and then drops off rapidly. The peak heat flux strongly depends on the thermophysical properties of chill, chill condition, superheat of casting and casting materials. Increased melt super heat and higher heat diffusivity of the chill material results in an increase in peak heat flux at the casting/chill interface. The presence of coating on chill material effectively reduces the peak heat flux. The heat flux curve in the case of coated chills is characterized by a double peak indicating re-melting of the solidified casting shell. The peak heat flux was modeled as a power function of dimensionless ratio which includes the thermal diffusivities of the chill and the casting materials, and pouring and liquidus temperatures of the solidifying casting material.The thermal plot of chill during solidification shows one dimensional heat flow at the initial stage and changes to two dimensional heat transfer. This was influenced by thermal conductivity of the chill material and heat capacity of casting. The heat transfer becomes one dimensional in the final stages. In coated chills heat flow was nearly one dimensional.

In coated chill experiments, HTC curve follows the same trend of heat flux transients. The second peak HTC value is lower for high thermal conductivity chill and higher for low thermal conductivity chill as compared to the first peak HTC. It indicates that solid shell formation and re-melting occurs in the case of higher thermal conductivity chill whereas in lower thermal conductivity chills, the re-melting of solid shell is absent. Contact angles of alumina coating estimated on various substrates indicated that the adhesion of the coating material on copper substrate was significantly better as compared to other substrate materials. The adhesion characteristics of the coating material affected the peeling of the coating from the chill surface and this influenced the time of occurrence of the second peak of heat flux transients. Metallographic analysis

indicated that higher thermal diffusivity of the chill and casting poured at higher superheat decreased secondary dendrite arms spacing (SDAS).

Keywords: *casting/chill interface, inverse heat conduction problem (IHCP), heat transfer coefficient, contact angle*

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F02

Modification Analysis of hypereutectic Al-Si Alloy with P or Phosphide by EET

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Aluminum phosphide (AlP) is the most effective modificator for the Al-Si system. To identify the modification mechanism, Based on empirical electron theory of solids and molecules (EET), in this paper, the valence electron structure of AlP unit cell was calculated. By comparing with the valence electron structure of Si, it was inferred that plenty of AlP particles generate as the reaction of pure P atom or Phosphide with Al atom in the Al-Si alloy melt, which has f.c.c structure and the distribution of electron space similar to primary Si phase, and the mismatching degree between AlP and Si structure is very small. From the calculation results we know the value of AlP is smaller than Si 鈥, so AlP particles precipitate firstly during the solidification processing, as the heterogeneous core of Si, and then the nucleation rate of Si is increased. The calculation results support for the classical theory of heterogeneous nucleation.

Based on the calculation method of interface valence electron structure (IVES), the IVES of (011) AlP/Si was calculated, and then the electron density of phase interface was obtained, whose value is 42.896%. The results show that there is no continuity on the interface (011) planes of AlP and Si, which indicated that the AlP particle on the (011) interface destroyed the preferential growth orientation of Si phase, and inhibited the Si crystal growth in the [011] direction, and then leaded to the refinement of Si phase. The valence electron structure determines, at least qualitatively, the micro-mechanism of Al-Si alloy modified by AlP particle.

F03

Numerical Simulation of Mold Filling and Solidification Process of a disc Aluminum Alloy in Pressure Die Casting

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The numerical simulations of mold filling and solidification process for the A380 aluminum alloy were done by the supposed mathematical model. The casting defects in the process of mold filling and solidification were predicted by the result of the casting simulation. The casting defects of simulation are well compared with the practice. Some measures presented were improved for the existing technological process.

Parts of casting process simulation are as follows:

Fig.1 Model of casting work

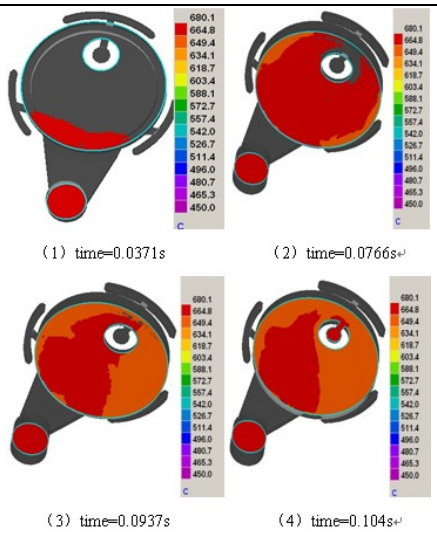

Fig.2 simulating results of casting process at different time

Keywords: *mold filling and solidification, numerical simulation, A380 aluminum alloy*

F04

Remelting Technology and Microstructural Evolution of Semi-solid Al-7Si-2RE Alloy

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In semi-solid remelting process, the various stages of reheating temperature and isothermal holding time must be accurately controlled in order to obtain the uniformly distributed and small equiaxed grains microstructure. In this paper, a temperature control program was developed and the remelting process for Al-7Si-2RE aluminum alloy was carried out. The results showed that with the raise of reheating temperature and the extension of isothermal holding time, the liquid fraction increases, α-phase grain grows and becomes rounding in the process of Al-7Si-2RE alloy semi-solid remelting. The most reasonable process parameters of reheating temperature is at 585~590℃ and its appropriate isothermal holding time is about 10~15min for the semi-solid Al-7Si-2RE alloy.

Keywords: *semi-solid; remelting technology; equiaxed grains; remelting*

F05

Numerical Simulation of Macrosegregation during Steel Ingot Solidification Using Continuum Model

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A continuum model is adopted to study macrosegregation phenomena that occur during solidification of large steel ingots. Evolution of temperature, melt velocity, and species concentration field during a 22-ton steel ingot solidification is illustrated by using the finite volume method. Numerical results of temperature distribution are validated by using experimental results. The influence of local permeability related to the friction that the melt experiences in mushy region is investigated. It is shown that the continuum model is able to predict the temperature field, and the variation of permeability obviously affects the melt flowing behavior and the final compositional distribution.

Keywords: *continuum model, steel ingot, macrosegregation, convection, permeability*

F06

Phase-field modeling of free dendritic growth in a binary alloy under a forced flow

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A phase-field model coupling with phase field, flow field and diffuse equation is presented for simulating isothermal dendrite growth of a nickel-copper alloy under a forced flow. Based on the finite difference method with uniform grid, the C Programming Code is implemented to complete the phase-field simulations. The simulation results indicate that the interfacial morphology, the symmetry of dendrite formation, tip growth velocity and the concentration distribution are crucially influenced by the fluid flow.

Keywords: *phase-field model, binary alloy, convection, dendritic growth*

F07

Micro-scale modeling of soft impingement during rheocasting

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The desired starting feedstock for semi-solid processing is partially solidified slurry in which the solid is present as fine and nearly perfect globular particles [1]. This curious microstructure has been of interest both commercially from enhanced mechanical properties and also scientific interest in explaining the mechanism of globular grain formation. Historically, the liquid is cooled down into the two phase regions by rheocasting processes, dendrites are formed and then, broken either through the bending of dendrite arms followed by liquid penetration of the high angle grain boundaries or through remelting at the root of dendrite arms due to direct or indirect agitation [1, 2]. Recent researches indicated that, if the initial grains were sufficiently high in number density, subsequent growth of these grains could be perfectly globular throughout the growth process [3].

In the present work, an attempt was made to give a generalized explanation of the formation and evolution of solidification microstructures in rheocasting, through a numerical model based on celluar automaton method for calculation of solid/liquid interfaces that are governed by solute diffusion and Gibbs-Thompson effect. Concentration at interface boundary is not described as boundary condition but its evolution is calculated through transport equations and a kinetic equation. The model was applied to Al-20wt.%Cu alloy, and was pursued by modeling of soft impingement problem and related to interface instability by constitutional supercooling theory. The results showed that the morphology of primary α-phase was determined by both the number of free crystals and the cooling intensity of melt. The presence of high density of nuclei and slower cooling of melt was responsible for the stabilizing effect on the morphological instability at the solid-liquid interface and promoted the globular growth of primary α-phase, which resulted from soft impingement of diffusion fields from adjacent growing crystals.

Keywords: *rhoecasting, soft impingement, microstructure simulation, cellular automaton*

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F08

Numerical Simulation of Structure and Shrinkage in Cast-steel Ingot

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By virtue of the numerical simulation software (FDM), this paper studied the influences of the ingot structure and insulation material to solidification and shrinkage of the ingot with 3-ton ingot as a sample. This research improved ingot structure and optimized process. In addition, the production outcome indicated that the optimized ingot and process planning can increase the finished product rate of the ingot.

Keywords: *Numerical Simulation, Structure, Shrinkage*

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F09

Simulation Study of the Effects of Parameters of Graphite Susceptor for Induction Metling Process of Polycrystalline Silicon

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Graphite susceptor and base plate play a key role in controlling the temperature of silicon melt in the induction melting of polycrystal silicon for solar cells. Different thickness and properties such as density, electrical conductivity of graphite susceptors could influence the heating effects of induction melting. An appropriate metling process of polycrystalline silicon is also closely related to parameters such as the material properties and the size of graphite susceptors. These parameters have great influence not only on the melting temperature of silicon melt but also on the efficiency of induction heating, impurity distribution, dendrite and the direction of crystalline grains, which ultimately affect the properties of the solar cells. Therefore, in order to obtain good quality and energy efficiency of growth of polycrystalline silicon, one needs to know how the temperature fields relate to the processing parameters such as different sizes and properties of graphite susceptors in the furnace.

To have a optimized control of processing parameters, A finite element based software COMSOL was used to simulate the temperature distribution of silicon melt in a poly-crystalline vacuum induction refining furnace. The simulation takes into account the interaction of the induced eddy current and the heat transfer coupling in the vacuum induction furnace. Some of the simulation results are summarized as follows:

1. The conductivity of the graphite susceptor has little impact on the temperature distribution.
2. The larger the amplitude or the higher the frequency, the sooner it reaches the melting temperature.
3. Base plate made of stainless steel 304 performed better than the copper base plate for the control of temperature distribution.

4. There exists an optimal thickness of the graphite susceptor, and the rise of temperature is not linearly proportional to the thickness of the graphite susceptor.

These simulation results are very useful for engineering to design a vacuum induction furnace and to understand relationship between the distribution of the electromagnetic field and the temperature field of the unidirectional solidification of silicon melt.

F10

Simulation of Sand Casting Production of Aluminium 13% Silicon Alloy

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With the advent of faster computer paralleled by the rapid development of numerical methods, the simulation of a manufacturing process becomes a vital tool as a part of the Computer Aided Engineering (CAE) system which relies heavily on cost effectiveness and quality. Prediction of casting defects associated with mould design can be done with tremendous speed using computational simulation. Such software can be utilised to optimise the design of product and casting system in the initial design stage to ensure good quality casting. In this paper casting simulation software ProCAST (based on finite element method) is used to simulate the production of sand cast slab of different thickness with. First model SAND1 has horizontal gating system, metal feeds through the horizontal plane, and the product cavity is horizontally positioned. The second model SAND2 has vertical gating, metal feeds through each section and the product cavity is vertically positioned. The simulation results show that model SAND1 has turbulent flow and the temperature distribution is not uniform throughout the cavity. The second design SAND2 filled with less flow turbulent from the bottom moving upwards. In the second model temperature distribution is relatively more uniform and good directional solidifictaion is attained.

Keywords: *Computational simulation, sand casting, mould design, turbulent flow, solidification, ProCAST*

f11

The establishment of some particular methods in casting simulation

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Cast simulation tool ADSTEFAN is useful to design casting technology of complicated iron castings. As an important reference, analyses of fluid, solidification and stress were carried out in routine work. Based on the function of solidification analysis, some special methods were determined to carry out the prediction and optimization of shake-out timing for large sized iron castings, the prediction of casting temperature distribution during heat treatment process and the prediction of residual stress in casting with using simple model. It was proved that these analyses are effective to iron casting production.

During the research of cast iron semi-solid process, to predict and control the influence of inclined cooling plate on flow and heat transmission of molten iron, on the basis of analysis model that has been built in this study. Flow field simulation considering temperature field is carried out by using casting simulating software for further research and satisfying with the practical production. Analysis model and a simulation result are shown in Fig.1 and Fig.2 respectively.

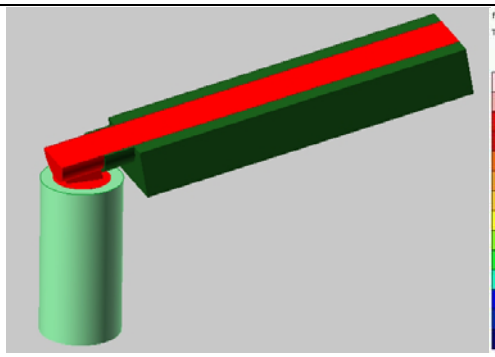

Fig.1 analysis model

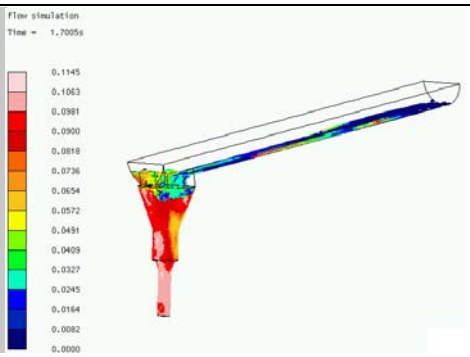

Fig.2 simulation result

Keywords: *Cast iron, Shake-out, Cooling plate, ADSTEFAN*

F12

Modeling on Directional Solidification of Solar Cell Grade Multicrystalline Silicon Ingot Casting

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Solar energy is considered as one of the best alternative energy in the future. Photovoltaic material is the core in this area. Multi-crystalline silicon ingot casting is the main production process for major supply of solar cell. However, the casting process cannot be understood clearly because of some difficulties, such as enclosed furnace, long cycle time of production and so on. In this paper, an integrated model, including casting process analysis, quality prediction and production parameters optimization, is proposed and the preliminary results were acquired. The framework of the proposed model will be introduced and the numerical simulation results on the temperature field, grain growth process are also given out and discussed.

Keywords: *Directional solidification, Multi-crystalline silicon ingot, Numerical simulation, Thermal control*

F13

Numerical Simulation of Fluid Flow Caused by Buoyancy Forces during Vacuum Arc Remelting Process

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The metallurgical structure and the component of ingots which depend critically on the fluid motion within the liquid molten pool during the VAR process have important effect on the machining process like forging, rolling and welding. In order to research the fluid motion of molten pool, a 2-D finite element model is established using ANSYS10.0 software, which combined models with the turbulent fluid flow and heat transfer. The fluid motion of the molten pool caused by thermo buoyancy forces is investigated at different VAR process in the present study. The results of this study have indicated that the fluid flows symmetrically along the axis of the molten pool, and flows along the clockwise circle at the right pool's profile. The results also show that the maximum velocity increases with the melt rate increasing. The relationship of the melt rate and maximum velocity is direct proportion.

Keywords: *Vacuum Arc Remelting, fluid flow, buoyancy forces, ANSYS10.0 software*

F14

Modeling and Simulation of Solidification and Temperature of Thick-wall Stainless Steel Pipe in Horizontal Centrifugal Casting Process

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A mathematical model of the horizontal centrifugal casting process based on the cylindrical coordinates for stainless steel casted pipe has been developed. Thermal boundary conditions, including the radiation and convection heat transfer conditions, have been taken into consideration due to the physical process. The model equation was solved numerically using non-uniform cylindrical grids and the finite differential method (FDM). Several parameters of cast process such as melt superheat, preheating temperature of mold, thermal conductivity of coating, which affect the temperature field and the positions of shrinkage porosity band to occur possibly in the solidification process have been investigated. The simulation results show that the positions of the shrinkage band will move obviously from the central region to inner region of casted pipe with increasing thermal conductivity of coating and reducing the convective heat transfer coefficient on the boundary of inner surface of casted pipe, while the effects of melt superheat and preheating temperature of mold are not so obvious, and that the thermal conductivity of coating has a great effect on the temperature field both of cast and mold.

Keywords: *centrifugal casting, temperature field, solidification shrinkage, numerical simulation, finite differential method*

G01

Modeling of Hydrogen Effect on Porosity Formation in Electron Beam Welded Titanium-based Alloys

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Electron beam welding (EBW) of titanium alloys have been studied in this work in order to identify the porosity formation mechanism which is prevalent. In this work a coupled thermodynamic/kinetic model for the diffusive mass transport of hydrogen in the heat affected zone and weld pool is developed. The modeling results indicate that hydrogen is likely to accumulate in the weld pool; coupling with a hydrogen diffusion controlled bubble growth model is used to simulate bubble growth. The complete model allows the prediction of the hydrogen concentration barrier for large pore formation. The effects of surface tension of liquid metal and the radius of pre-existing micro-bubble size on the barrier are discussed. The hydrogen diffusion-controlled bubble growth model provides the framework for future research for bubble growth in the weld pool.

Keywords: *Titanium welding, Electron beam welding, Hydrogen porosity.*

G02

High temperature indentation test to improve constitutive model for welding simulation

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The very concentrated heat input during fusion welding, leads to a local dilatation and metallurgical transformations that generate inhomogeneous plastic deformation, residual stresses and distortions in the welded parts which can be a source of cracking and fracture problems in welded structures. To predict such residual stresses and distortions, finite element analysis is nowadays widely used. The aim of this work is to develop a 3D finite element model for welding simulation. The proposed model is based on semi coupled thermo-mechanical analysis using a double ellipsoidal model of heat source. For a first level of validation, the problem of a disk heated in its central zone is investigated. The second level of validation concerns the simulation of a fully 3D two pass butt weld. The key findings of this work concern the calibration of the heat source parameters with the help of the inverse analysis to improve the heat flow predictions. For the stress analysis, an annealing temperature is introduced to force the material to lose its hardening memory above a given temperature. The predicted residual stresses as well as the predicted distortions are found to be sensitive to the annealing temperature.

Keywords: *Welding, Finite element, Residual stress, Inverse analysis, Annealing temperature*

G03

Control of root pass stress by two-sided arc welding for thick plate of high strength steel

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For thick plate of high-strength steel, it is extremely important to control of residual stress. A new method for thick plate which does not require back gouging – two-sided arc welding – is adopted to control stress. Root pass adopts asymmetrical two-sided gas tungsten arc welding with wire feed in vertical up welding. The key of controlling stress for this method is to determine the arc distance and welding parameters of two-sided arcs. The effects of arc distance between fore and rear torches and heat inputs on the stress are investigated through experiments and numerical simulation. The calculated results are in a good agreement with the experimental results. The influence mechanism on welding stress of the arc distance and heat input is obtained. Research results show that selecting proper arc distance and regulating heat input of two arcs control effectively stresses.
Keywords: *Numerical simulation, high strength steel, thick plate, Stress controlling, two-sided arc welding*

g04

The Effect of Post Heating on Nugget Quality for Spot Welding Dual Phase Steels using FE and Experimental Method

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Advanced High Strength Steels (AHSS) will become increasingly common in future automobiles, due to ever stricter crash safety and fuel consumption requirements. As a consequence different technologies for their joining are studied. Currently, the most common joining technique in automotive industry is resistance spot welding. And this will remain to be the case in the foreseeable future. Consequently, a deep research into the weldability of AHSS is needed. This paper presents the results of an numerical model and experimental evaluation of the post heating on the microstructure and weld strength of dual phase (DP) advanced high strength steel.
The paper presented a basic analysis of the effects of post heating on the quality of the resistance welds in dual phase advanced high strength steels based on FEA method and experimental investigations. It was shown that post heating can significantly improve the weld strength and maximum displacement of the welds. Based on the analytical results it can also be concluded that too large post weld current and too long post weld time don't help to improve the quality of the weld. Therefore an assumption can be made, that the energy input during post heating phase is important for the weld quality.
Keywords: *Dual phase steels, Spot welding, Numerical model, Post heating, Weld quality*

G05

Effect of rotation speed on the temperature field and axial shortening of inertia friction welded GH4169 joints by numerical simulations

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A two-dimensional finite element model was established for inertia friction welding of GH4169 superalloy based on the ABAQUS environment. The remeshing and map solution techniques were adopted to solve the problem of element distortion. The effect of rotation speed on the temperature field and axial shortening of joints was investigated. The results show that the interface temperature increases rapidly to more than 900 °C within a second. And then, it increases slowly to a quasi-stable value. The axial shortening begins to augment quickly when a uniform interface temperature field has been formed and the plasticized material is extruded from the interface to form an obvious flash. The rotation speed of the flywheel controls the welding process and has a significant influence on the temperature evolution and axial shortening of joints.

Keywords: *Inertia friction welding, Numerical simulation, Map solution, Temperature field*

G06

Finite element model for the bonding process of anisotropic conductive films joints

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The use of anisotropically conductive film (ACF) for the direct interconnection of flipped silicon chips to printed circuits (flip chip packaging), offers numerous advantages such as reduced thickness, improved environmental compatibility, lowered assembly process temperature, increased metallization options, cut downed cost, and decreased equipment needs. The most common chip-on-glass (COG) interconnections technology currently used in display applications is based on anisotropic conductive film (ACF) [1-3]. The principle of COG bonding using ACF is that the electrical connections are established through conductive particles and the mechanical interconnections are maintained by the cured adhesive. The size of the contact area and the shape of the conductive particles are important factors in determining conductivity.

In this study, the bonding processes of COG (Chip-on-Glass) assemblies are investigated by finite element analysis and experiments. One damage model for the conductive particles was developed within this finite element model. The results show that the effects of bonding parameters (bonding temperature, bonding pressure and bonding time), properties of the substrate, ACF materials and the conductive particles on the reliability are significant. Additionally, the effects of bonding parameters on the damage of the conductive particles are obviously, which are useful to industry.

Keywords: *anisotropically conductive film, chip-on-glass (COG) , Finite element model*

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G07

3D transient thermal modelling of the temperature profile during laser assisted machining of Ti6Al4V alloy

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Titanium alloys have been widely used in the aerospace, biomedical and automotive industries because of their high strength-to-weight ratio and superior corrosion resistance at room and elevated temperature [1]. However, titanium alloys are difficult to machine due to their high strength, low thermal conductivity and high chemical reactivity. This means that conventional machining of titanium alloys is a low productivity process with high materials running costs [2]. Laser assisted machining (LAM) offers ability to machine difficult to cut materials more efficiently and economically [3]. Normally, measurement of temperature variation during laser surface treatment is not possible due to the high temperature variation rate. The aim of this work is to develop 3D transient finite element model to predict 3D temperature distribution in Ti6Al4V workpiece, optimize the laser parameters and tool position during LAM process. The simulation results are compared with the results produced by experimental work, showing good agreement. The influence of laser parameters on the temperature distributions in the Ti6Al4V alloy workpiece was also investigated, which provides important information to optimize and improve the LAM technique.
Keywords: *Laser assisted machining (LAM), 3D transient finite element model (FEM), Ti6Al4V alloy, 3D temperature distribution*

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g08

Finite element Method application for modeling of PVD coatings properties

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The aim of the research is the computer simulation of the internal stresses in bilayer coatings Ti+TiN, Ti+Ti(CxN1-x), Ti+TiC obtained in the magnetron PVD process on the sintered high-speed steel of the ASP 30 Computer simulation of stresses was carried out in ANSYS environment, using the FEM method and the experimental values of stresses were determined basing on the X-ray diffraction patterns.
The computer simulation results correlate with the experimental results. The presented model meets the initial criteria, which gives ground to the assumption about its usability for determining the stresses in coatings, employing the finite element method using the ANSYS program. In order to evaluate with more detail the possibility of applying these coatings in tools, further computer simulation should be concentrated on the determination of other properties of the coatings for example micro-hardness.
Presently the computer simulation is very popular and it is based on the finite element method, which allows to better understand the interdependence between parameters of process and choosing optimal solution. The possibility of application faster and faster calculation machines and coming into being many software make possible the creation of more precise models and more adequate ones to reality

Keywords: *Analysis and Modeling, Computational Materials Science, Finite Element Method, Stresses, Coatings PVD*

G09

Deposition conditions effect on TiN film growth by molecular dynamics simulations

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With good resistance to high temperature, wear and corrosion, TiN coatings have found their uses in applications such as cutting tools and many mechanical components. The properties of coatings are determined by their atomic structures. Because of the complexity of vapor deposition, increasing reliance is placed upon modeling to achieve the needed atomic scale control. In this study molecular dynamics simulations using the modified embedded-atom method (MEAM) potential have been used to investigate the growth mechanisms of TiN films from thermalized atomic titanium and nitrogen fluxes. The crystallinity and stoichiometry of the deposited crystal structures were determined as a function of growth temperature and Ti:N flux ratio. The best deposition condition of TiN coatings was proposed.

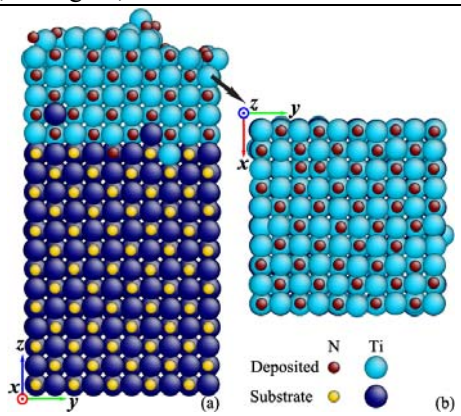

Fig. The morphology of TiN film deposited on TiN(001) substrate.
(a) side view, (b) top view from 4th deposited layer

Keywords: *molecular dynamics, TiN, vapor deposition, modified embedded-atom method*

G10

The Analysis of stress and strain field of the laser cladding process on the ring circular orbit

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The cracking of coatings and the deformation of base frustrated the application of the laser cladding technology especially on surface of the ring circular orbit. As an important factor for the two problems above, the study of the stress and strain promotes this technology's application. The stress and strain field of the laser cladding process on the ring circular orbit was analyzed trough the finite-element method. The wedge module of the ring circular ring was the subject investigated and the stress and strain field was solved based on the temperature field. The calculating result shows that during the cladding process on the ring circular orbit the crank point tends to generate the transversal crack; the centre point on the interface of the coating and base tends to generates longitudinal crack; the intersecting edge of the coating and base tends to generate toe crack. Moreover, the cracking tendency of the outer marginal point is obviously larger than that of the inner marginal point. The rather large stress appears at the border position where the constraint is placed on, the stress on the point before the cladding layer under the range of irradiation is large as well. And the displacement becomes larger as the cladding process proceeds.

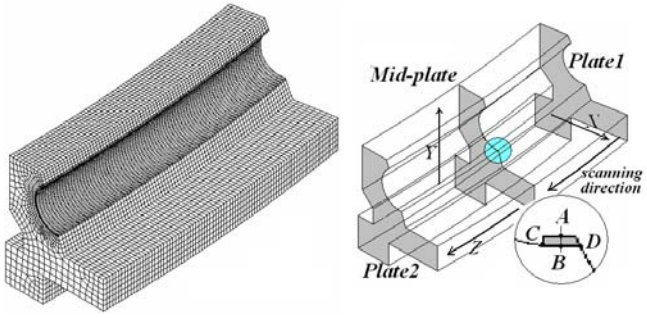

Fig1 The sketch map of griddling of the wedge module of the ring circular orbit and selected points

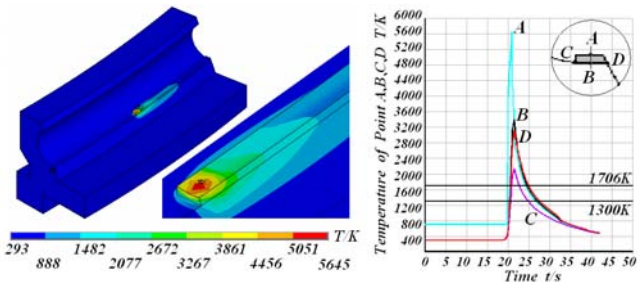

Fig2 The temperature distribution map at the 21s and the temperature variations at Point A, B, C,D and D

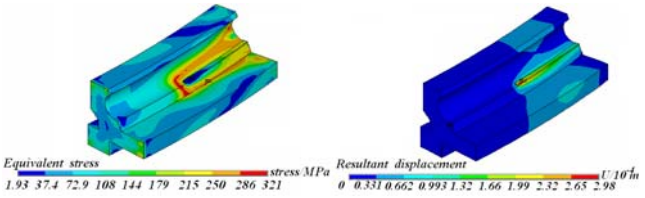

Fig5 The equivalent effective stress distribution map and the displacement distribution map at the 21s

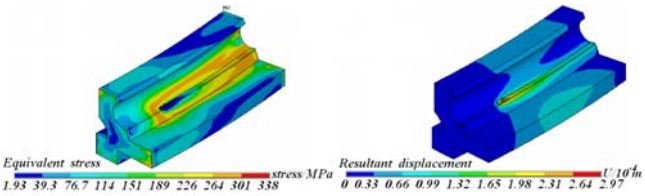

Fig6 The equivalent effective stress distribution map and the displacement distribution map at the 31s

Table 1 The residual stress and plastic strain at A, B, C and D at the 50s

	Direction	*X*	*Y*	*Z*
A	Plastic strain /10-2	-0.3	-0.8	1.1
	Residual stress /MPa	50	100	250
B	Plastic strain /10-2	-0.3	0.4	-0.01
	Residual stress /MPa	55	50	320
C	Plastic strain /10-2	0.3	-0.2	-0.01
	Residual stress /MPa	10	40	300
D	Plastic strain /10-2	1.2	-0.7	-0.4
	Residual stress /MPa	25	-65	250

Keywords: *Laser cladding, circular orbit, stress and strain field*

G11

Three-dimensional numerical simulation of splat formation on substrates with different conditions in plasma spraying

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Plasma sprayed coatings are built up by the accumulation of splats formed by the impacting, spreading and solidifying of individual molten droplets on the substrate. In the present work, a three-dimensional computational model including heat transfer and solidification is established to simulate the formation process of a single splat using the computational fluid dynamics (CFD) software, Fluent. The fluid flow and energy equations are discredited and solved according to typical finite volume method on an unstructured grid. A volume of fluid (VOF) tracking algorithm is used to track the droplet flow with free surface. In order to understand the splat formation mechanism, the process of splat formation by a molten nickel droplet impacting and spreading on a polished mild steel surface was simulated. On this basis, the simulations of impact of a molten droplet on substrate with different conditions including substrate surface morphologies, substrate thermal conductivity, substrate initial temperature and thermal contact resistance were presented. The simulation results clearly show the effect of different substrate conditions on the shape of the final splat and splash behaviors.

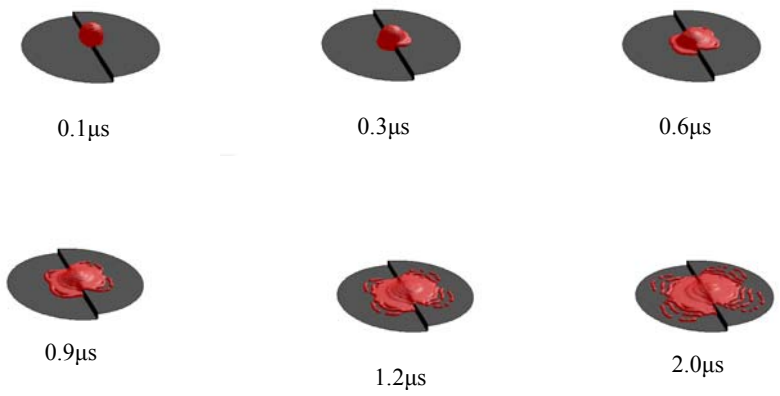

Fig. 1 Simulations showing the splat formation process of a 60 μm diameter molten nickel droplet at 2000 k impacting with a velocity of 100 m/s on a mild steel edge initially at a temperature of 300 k.

Keywords: *numerical simulation, splat formation, plasma spraying, molten droplets*

G12

Structures and properties of VC coating on Cr12MoV cold working die surface steel by TD process

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VC coating was prepared on the surface of Cr12MoV cold working die steel with Thermal Diffusion (TD), and its micro-structures, energy spectrum, hardness and bonding strength were measured with Scanning Electric Microscope (SEM), Energy Dispersive Spectroscopy (EDS), micro-hardness tester and scratching tester, respectively, and the forming mechanism of VC coating was analyzed. The experimental results are shown that the coating structure is a even and fine single-phase, it micro-hardness is 3050HV; the bonding form is metallurgical combination, its bonding strength is 47.1N by scratching method, that is benefit to increasing fatigue life of cold working die.

Keywords: *TD process; vanadium carbide coating; bonding interface; surface morphology*

Financial support of this research by the Natural Science Foundation of the Jiangsu Higher Education Institutions of China (Grant No.08KJB430002) and the Technique Innovation Program of Changzhou, China (Grant No.CN20090023), is gratefully acknowledged.

g14

Molecular dynamics simulation of bonding at the Fe-Al interface

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Molecular dynamics simulations was performed using Nose/hoover temperature thermostat ensemble to investigate bonding between Fe (0 1 0) facet and two Al facets of (0 1 0) and (1 1 1). The detailed trajectory analysis reveals that Al lattices rotate at the Fe-Al interface during annealing at the temperatures ranging from 100K to 900K. The lattice rotation is a process of energy minimizing and the rotated layer is largely depended on the annealing temperature, annealing time, and annealing heating-up rate. With the increase of annealing temperature, more layers rotate in the Al domain, while the Fe atoms remains their original crystallographic orientations. With the increase of annealing time and heating-up rate, more layers also rotate in the Al domain. The calculated equivalent stress shows that different Al orientations cause different levels of stress at the interface of Al-Fe system.
Keywords: *Molecular dynamics, Fe-Al, bonding, lattice rotation*

g15

Effects of Crack Opening Angle and External Loads on the Reliability of Welded Pipe with Circumferential Crack

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In this paper, the reliability of welded pressure pipe with circumferential surface crack was calculated by using three dimensional stochastic finite element method. This method has overcome the shortcomings of conservative results in safety assessment with deterministic fracture mechanics method. The calculation of reliability was based on three dimensional elastic-plastic stochastic finite element program which was developed by ourselves. The effects of variables such as fracture toughness, bending moment and the depth of the circumferential surface crack on the structure reliability were also discussed. The calculation results indicate that the crack opening angle has certain effect on the reliability of the welded pipe. When the mean value of bending moment is 10000N.m, with increasing the crack opening angle from 30o to 180o, the failure probability of the welded pipe will change from 3.8379×10-8 to 3.6943×10-6. When the mean value of bending moment is 15000N.m, with increasing the crack opening angle from 30o to 180o, the failure probability of the welded pipe will change from 3.9865×10-6 to 1.9367×10-3. The bending moment has great effect on the reliability of the welded pipe. When the mean value of moment is changed from10000N.m to 15000 N.m, the failure probability of the welded pipe increases dramatically for the same circumferential crack opening angle. Irrespective of the changing of moment, the pipe has higher reliability if the crack opening angle is less than 60o. The method has put forward a new way for safety assessment of welded pipe with circumferential surface crack.
Keywords: *welded pipe, circumferential surface crack, stochastic finite element method, reliability, safety assessment*

g16

Modeling of the whole friction stir welding process by the explicit finite element method

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A fully coupled thermo-mechanical three-dimensional finite element model was developed for the friction stir welding (FSW) process in the ABAQUS environment using the Johnson-Cook material law and Johnson-Cook failure model. The temperature evolution during the plunge, dwell and moving stages of FSW 7050 alloy and the effect of heat conduction by the back plate were investigated. Results show that the temperature almost symmetrically distributes across the plate cross-section and the temperature contour in the weld nugget zone presents a V-type shape after the plunge stage. In the dwell stage, the frictional heat conducts around to preheat the plate. While in the moving stage, the heat gradually accumulates until a quasi-stable temperature field is formed. Moreover, the heat conduction through the back plate has significant effect on the temperature field. With increasing the heat convective coefficient of the back plate the temperature field is remarkably compressed.

Keywords: *Friction Stir Welding; 7050 Aluminum Alloy; Explicit Finite Element Analysis; Temperature Field*

g17

Numerical Simulation of Semisolid Die Casting Process of Magnesium Alloy

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A 3-D mathematic model of rheo-forming mould-filling coupled with semi-solid magnesium alloy apparent viscosity was established. The flow characteristics of liquid filling comparing with those of semi-solid filling were analyzed. The results indicate that the liquid filling has turbulent flow characteristics, while the semi-sold filling has laminar flow characteristics which can reduce the foundry defects such as gas cavity and oxidation mixture. The distribution of pressure reduced gradually in the filling direction during semi-solid filling process which would generate back pressure that was favorable for filling process. And the simulation results were in accord with the experimental results. The high quality castings could be obtained through semi-solid rheo-forming.

Keywords: *numerical simulation, semisolid, magnesium alloy*

g18

Analysis of Temperature－Stress Coupling Field in Laser Cladding Process with Powder Feeding

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The three-dimensional transient physics model of temperature-coupling field in laser cladding process with powder feeding was constructed based on ANSYS software. The simulate process of Ni alloy powder laser-cladding on steel 34CrNi3Mo also been calculated. The method of birth-death element was used to simulate the reaction between powder and molten pool both at before and after the pool was formed, the free surface shape of molten pool and temperature-stress coupling field were obtained. The calculate results match with the results of experiments well which proves the constructed model is correct and reasonable.

Keywords: *Laser cladding, birth-death element method, transient temperature field, Coupling field, 34CrNiMo*

G19

Notched Tensile Fracture of Ti-15V-3Cr-3Sn-3Al Alloy

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Notched The notched tensile strength (NTS) and fracture toughness of Ti-15V-3Cr-3Sn-3Al (Ti-15-3, metastable β Ti alloy) specimens that were aged at different temperatures were determined. The ultimate tensile strength of the aged specimens varied in the same manner as the hardness, but inversely with ductility. The specimen aged at 371oC (under-aged specimen) was the most susceptible to notch brittleness among the specimens. An obvious rise in NTS was obtained with specimens aged at 538oC or higher. The change in fracture toughness of the aged specimen was consistent with the variation in the NTS, i.e., both the fracture toughness and NTS increased with an increase in aging temperature. The notched tensile test could be used to evaluate the relative resistance to crack growth of the materials, instead of using the complicated fracture toughness method.

Keywords: *Notched tensile strength; Ti-15V-3Cr-3Sn-3Al; Fracture toughness.*

G20

Effect of Solution Annealing in Post and Preheat Conditions on Microstructure and Mechanical Properties of IN-718 Weld Metal

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Inconel 718 is precipitation hardening Nickel base alloy. This alloy has combination of corrosion resistance and high strength with outstanding weld ability, including resistance to postweld cracking. The IN 718 has excellent creep-rupture strength at temperatures up to 700 .This alloy obtains to desired precipitation of γ', γ'' and δ phases during heat treatment for control grain size and strength[1].Mechanical properties of Inconel 718 can be achieved by choosing proper heat treatment. The precipitation hardening is used for control of IN 718 microstructure. The process consists heat treatment is required to ensure proper rate between γ'' and δ phases[2].Laves phase, which forms as a result of segregation, is an important aspect of IN 718 weld metal. However, when the Gas Tungsten Arc Welding(GTAW) process is used, micro-cracking may occur in the Heat Affected Zone(HAZ)[3].The welding of this alloy carried out in solution annealed conditions, followed by ageing heat treatment, which combines stress relief with development of the strengthening phases[4].

In this investigation the mechanical properties and microstructure of IN 718 weld metal were studied. four samples were prepared in different conditions as:

a- Solution annealing in $970^{o}c$ for 60 minutes before welding.

b- Solution annealing in $970^{o}c$ for 60 minute before welding and direct aging in $720^{o}c$ for 480 minutes after welding.

c- Solution annealing in $970^{o}c$ for 60 minutes before welding and then solution annealing with aging after welding.

d- Solution annealing and aging before welding.

The mechanical test result showed that high tensile strength of weld metal gained in "C" condition, SEM and optical metallographic result showed that different volumetrically γ' and Lave phase provenance of different mechanical properties of weld metal.

Keywords: *heat treatment,IN-718,TIG weld*

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H01

Numerical analysis of a railway brake disc

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A certain number of railway brake discs, made of gray cast iron, shown the presence of small cracks only after a few thousand kilometers. To investigate main causes of a brake disc failure, numerical analysis was done, using ABAQUS software. Numerical analysis resulted from a physical model of heat flux in dependence of braking time. Physical model was applied considering all demands and presumptions given by industry representatives.

Keywords: *railway brake disc, thermo-mechanical analysis, numerical analysis, re-design*

H02

Numerical analysis of braking discs for a »Taurus« class locomotive

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This paper shows thermal-stresses numerical analysis of the brake discs for a »Taurus« class locomotive. »Taurus« class's locomotives brake with the brake discs mounted on a »brake shaft«, which is driven from the drive axle through a gear pair, which is shown in Fig. 1, left and marked with the dot line. The engine consists of two trolleys with two drives in one cart.

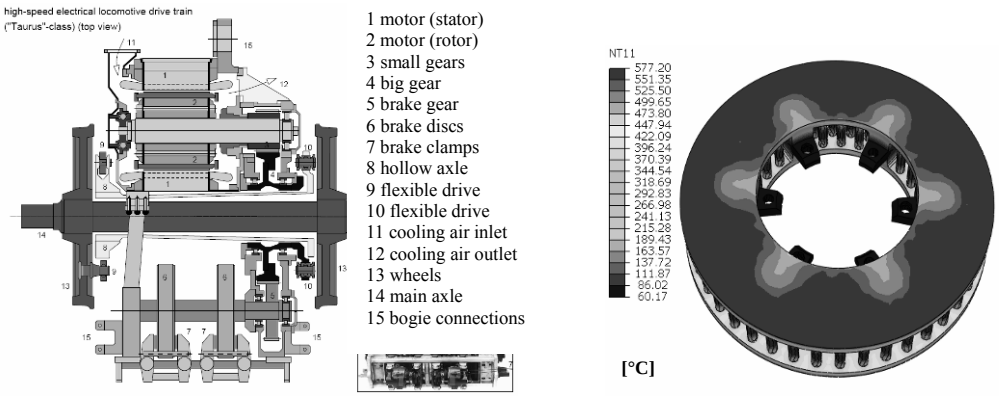

Fig. 1: Brake system locomotive »Taurus« and temperature field of brake discs after last braking

The numerical analyses (temperature and stress) were carried out under the experimental testing program »Prüfprogramm Nr. 5« in multiple steps, suited for this type of locomotive with two braking; from 240 km/h to 160 km/h and from 160 km/h to standstill. In each step different boundary conditions (wet –, dry – sintered braking pads with a friction coefficient of 0.4), were considered.
The main boundary condition (a physical model) in the thermal-stresses numerical analysis is the heat flow in relation to braking time (Eq. 1.) into the brake disc, which can be written with the following expression:

$$P_i = 2 \cdot F_i \cdot \mu_B \cdot \frac{r_B}{r_K} \cdot i \cdot v_i \ \text{[W]} \qquad (1)$$

Numerical analyses were carried out using the finite element method (FEM) and the software package ABAQUS CAE 6.7.1. In the Fig. 1. (right), one example of a temperature field of brake discs after last two-step braking, is present. The maximum value of temperature was 577 °C.

Keywords: *locomotive »Taurus«, the brake disc, thermal and stresses analysis*

H03

Mathematical modeling and simulation of lime burning process in a normal shaft kiln

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In this research, a mathematical model is established to investigate heat and mass transfer as well as chemical kinetics, especially gas and solid temperature profiles associated to lime burning process in a normal shaft kiln. The transport of mass and energy of gas and solid phase is modeled by a system of differential equations with solving boundary value problem. Besides a shrinking core approach is employed to study the mechanics and chemical reactions of the solid material. The influences of energy input, limestone origin and particle size distribution including pressure drop to the lime burning process are considered. The decomposition rate of limestone are experimentally carried out in laboratory and these results are in good agreement with those calculated from simulations.
Keywords: *Shaft kiln,, lime burning, modeling and simulation, heat and mass transfer, temperature profile*

H04

Phase diagram simulation and heat-treatment of a Ni-based alloy for high-temperature vitriol pump

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To develop a Ni-based alloy for high-temperature vitriol pump which is submitted the corrosion of vitriol and rush of liquid with solid particles, the equilibrium phase diagrams of some Ni-Cr-Fe-C-Mo-Si-Cu alloys were calculated by Thermo-Calc. The chemical composition of a new Ni-based alloy was proposed based on the simulation results and the mechanism of sigma phase precipitation strengthening. The alloy was casted and heat-treated. Some ageing treatments were carried out at 973K, 1023K, 1073K, 1123K for 4h. It was investigated the phases by XRD, the microstructures by OM and SEM, the chemical compositions by EDAX. The proposed alloy consists of γ, σ and $M_{23}C_6$ from 1073K to 1273K. The most amount of σ phase is up to 12.45 % (mass) at 1023K, it decreases with the augment of equilibrium temperature. It disappeared above 1323K. The amount of σ phase is enough in alloy to supply good precipitation hardening at a large temperature range. Experimental results were compared with the results of phase diagram simulation by Thermo-Calc. The alloy can be effectively strengthened by sigma phase precipitation at the temperature from 1023K to 1073K. Experimental results verified the validity of phase diagram simulation. Thermodynamic phase diagram calculation could be one of effective tools for alloy design, it can offer appropriate guidance for the materials design and reduces the amount of experimentation.

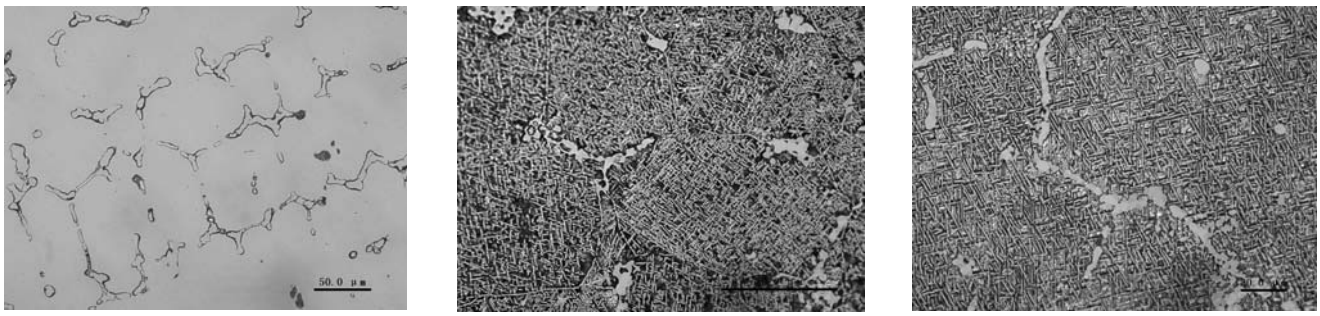

Figure 1. Microstructure of Ni-based alloy, (a) as casted, (b) aged 4h at 800℃, (c) aged 4h at 850℃

Keywords: *Ni-based alloy, vitriol pump , precipitation strengthening, phase diagram simulation, aging*

H05

Optimization of pellet production process parameters in grate using simulation results

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The objective of the paper is to optimize the parameters of pellet drying and preheating process in grate. A mathematical model of drying and preheating is developed, and is verified by the experiments. Further, the operating parameters of wind temperature, wind speed, grate speed and bed depth etc. are investigated through orthogonal method using the simulation results. And a relationship between drying, preheating effects and operating parameters is achieved. The results show that the optimization effect can be achieved in the given range when air velocity is about 3.0m/s and temperature is about 300℃, 500℃, 800℃, and 1100℃ in the updraft drying zone, downdraft drying zone, preheating I zone, and preheating II zone respectively. The work is help to save energy and reduce emissions in pellet induration.

Keywords: *grate, drying and preheating, orthogonal method, pellet, experiment*

[This work is fully financed by the National High-Tech Research and Development 863 program of China under Grant No.2007AA05Z215.]

H06

Optimization of Pellet Induration Process Parameters in Rotary Kiln Using Simulation Results

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In order to optimize the pellet induration process parameters of the rotary kiln, the mathematical model is developed and solved with commercial software FLUENT. Orthogonal regression has been performed by using the simulated results of the pellet induration in rotary kiln. The functional relations between pellet induration quality and process parameters are obtained. The main parameters that affect the thermal process are also discussed. The results show that the high-temperature zone is longer and the local high-temperature could be avoided while the velocity difference decreasing between the secondary air

and the carbon particle, which leads to more uniformed temperature distribution and better induration quality. The work gives a right direction on improving of pellet production.

Keywords: *rotary kiln, pellet induration, optimization, orthogonal regression*

[This work is fully financed by the National High-Tech Research and Development 863 program of China under Grant No.2007AA05Z215.]

H07

Development and application of Thermal Mathematical Model of iron ore pellet bed in grate

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On the analysis of heat transfer mechanics, physical and chemical change of pellet drying and preheating process in grate, the mathematical model is established and solved by three-diagonal matrix algorithm. With Visual Basic 6.0 the simulation software is developed. The model is verified by measurements at a domestic pellet plant, and the temperature distribution of pellet bed is gained. Meanwhile, the influence of different operation parameters on the pellet thermal process are studied, the results can be taken as a basis of practical production control and the grate optimizing design.

[This work is fully financed by the National High-Tech Research and Development 863 program of China under Grant No.2007AA05Z215.]

Keywords: *iron ore pellet, grate, thermal process, mathematical mode, simulation*

h08

Evaluation model of susceptibility to hot shortness of Cu-containing LC steel

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It is well known that copper causes the hot shortness problem when in the scrap based steelmaking process. Hot shortness occurs because of selective oxidation of the iron whereby the more noble copper is enriched at the steel-oxide interface and embrittlement take places during hot working. In this paper, in order to control the Cu hot shortness, the evaluation model of susceptibility to Cu hot shortness was investigated. Here, several specimens with copper contents (0.13 to 0.38wt%) and nickel contents (0.05 to 0.13wt%) were prepared, the oxidation test was performed at 1100, 1150 and 1200°C and hot compression test were conducted at 1150°C using a Gleeble 3500 to examine the Cu induced surface cracking. The aim of this work is that an evaluation model is derived to express the hot shortness susceptibility in terms of Cu enrichment characteristics. We found that Cu hot shortness susceptibility is related to the oxidation rate, the copper equivalence and the scale-steel interface length ratio. Also, it is founded to exist a fairly nice correlation between the oxidation rate and other factors such as chemistry elements, oxidation conditions, especially the Ni content.

Keywords: *Cu hot shortness, Oxidation rate, Copper equivalence, Crack susceptibility*

H09

Nanoscale mechanical behaviors of nanostructured silicon

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Molecular dynamics (MD) simulation is adopted to examine the deformation behavior and phase transformation of mono-crystalline SiNW subjected to tensile force. The techniques of coordination number (CN) and centro-symmetry parameter (CSP) are used to monitor and elucidate the detailed mechanism of the phase transformation throughout the whole process in which the detailed evolution of structural phase change and the dislocation pattern can be identified. Therefore, the relationship between phase transformation and dislocation pattern can be established and illustrated. Moreover, the electrical resistance and conductivity of SiNW can be evaluated by using the concept of virtual electric source. The change of electrical resistance is then annotated at the same time. Moreover, the effects of the stress release and temperature on the structural phase transformation of mono-crystalline SiNW for three different crystallographically oriented surfaces are investigated. Simulation results show that: before the failure of the material, the dislocations are introduced first and then the phase transformation will be formed with a view to minimizing the total energy of the system. For (011)- and (111)-oriented SiNWs, the electrical resistance can be altered only as the stress level is higher than yield strength. For (001)-oriented SiNW, however, its electrical resistance can be changed even at stress level lower than yield strength. As the stress level reaches to the level of 24 GPa, a significant amount of metallic Si-II and amorphous phases will be formed from original semiconducting Si-I phase and lead to a pronounced decrease of electrical resistance. Finally, it is found that as the temperature of system is higher than 500 K, the electrical resistance of SiNW can be efficiently reduced through the process of axial elongation.
Keywords: *Si nanowire, Molecular dynamics, Phase transformation, Mechanical properties, Tensile force, Electric resistance.*

H10

High Temperature Mechanical Properties of a Ti-microalloyed Complex Phase Steel

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With Gleeble-3500 thermomechanical simulation testing machine, the effect of different temperature (between 700°C -1450°C) and strain rate on high temperature mechanical properties of Ti-microalloyed complex phase steel (CP steel) specimens was investigated. The experimental results showed that between 800°C -1150°C, with the same test strain rate, the tensile strength(TS) of the investigated steel increases with the test temperature decreasing. On the other hand, at the same test temperature, TS increases with the strain rate increasing. The highest stress of 252 N/mm2 is obtained at 800°C. All of the area reduction(AR) values are fairly good in the tested temperature range of 800°C -1450°C.
Keywords: *Ti-microalloyed complex phase steel; high temperature mechanical properties; tensile strength; area reduction; strain rate*

H11

Thermo-Elasto-Plastic Damage Analysis of Functionally Graded Materials under Thermal Loading

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Functionally graded materials（FGMs）are developed with the purpose of alleviating or eliminating thermal residual stress due to interface mismatch between dissimilar materials, such as metals and ceramics. Considering that the processing or/and suffering condition are usually under thermal shock or thermal cycle, the thermo-elasto-plastic damage analysis of this class of material is necessary and important for the stability of the whole structure and service life.

It was verified in Jae-Myung's research[1] that the finite element method based on continuum damage mechanics was feasible for elasto-plastic damage analysis of FGMs under thermal shock and thermal cycle. It was discussed on one side, the effects of the distribution of thermo-elasto-plastic properties on initiation position and time of damage, however, on the other side, the influence of damage on thermal and mechanical properties were not considered. The essential reason for the shortcoming of Jae-Myung's work is that the definition of damage has no micro-structural basic. Focused on this, the volume fraction of voids is considered to be damage in micro-scale. Lemaitre's damage model[2] is also employed to analyze the damage behavior of FGMs subjected to thermal loading. The volume fractions of constitutions are assumed to change continuously in the thickness in the style of power function. The material parameters contained in the constitutive equation and damage evolution equation are assumed to be functions of temperature, and the spatial variation on thickness direction is calculated through mixed rule. Considering the calculating cost, the isoparametric graded finite elements [3~5] are used. By calculation procedure of finite element formulation, the influence of volume fraction of voids and its distribution on the thermo-elasto-plastic properties of functionally graded materials under thermal loading is discussed. The functionally graded structure is optimized by comparing damage evolutions of different functions of volume fraction distribution.

Keywords: *functionally graded materials, thermo-elasto-plastic damage, voids, temperature relativity, thermal loading*

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H12

Properties and electronic structure of iron under pressure up to 30GPa

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The properties and electronic structure of Fe under pressures of 0-30GPa have been studied by first principles employing density functional theory (DFT), ultra-soft pseudo-potentials (USPP) and the generalized gradient approximation (GGA). The calculated results show that there is a structural transition from magnetic bcc to nonmagnetic hcp structure for Fe around 11GPa. There is a pseudogap both in the density of states (DOS) for bcc and hcp Fe. The pseudogap of bcc Fe is deeper and wider than that of hcp Fe. The elastic modulus was obtained by Voigt-Reuss-Hill averaging scheme. The results indicate that the elastic properties of bcc Fe enhance with pressure except for C11, shear modulus G and Young's modulus E at the transition pressure, while the elastic properties of hcp Fe increase linearly with pressure. Bcc Fe is ductile, and hcp Fe becomes ductile from brittle around 25GPa.

Keywords: *iron, mechanical properties, electronic structure, ab initio calculations*
Supported by the National Natural Science Foundation of China (Grant No.50871035) and Ph.D. Programs Foundation of Ministry of Education of China (Grant No.20060213017)

H13

Numerical Simulation of Defect Inspection Using Electromagnetic Stimulated Thermography

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The feasibility of electromagnetic stimulated thermography non-destructive testing for the detection of defects in metallic conductive materials has been carried out by finite element analysis. An aluminum plate with defects of different diameters, depths, locations, shapes and orientation with respect to eddy current was numerically investigated. ANSYS software was used to solve the coupled electromagnetic and temperature field equations. The peak temperatures on the top surface of circular defects with different diameters and depths were calculated on varying excitation frequencies. It was demonstrated that the obtained temperature was proportional to the defect diameter and depth. The dependence of the temperature over the top surface of the defect on its location and orientation was also presented. The results indicate that we can detect the subsurface defect and estimate its depth and location by choosing a suitable coil-specimen configuration.

Keywords: *numerical simulation, electromagnetic, thermography, non-destructive testing*

H14

Numerical Simulation of the NDT of Metallic Composites Plate by Infrared Thermography

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This paper aims to the Non-Destructive Testing(NDT) of debonding in Metallic Composites Plate(MCP) by Infrared thermography, Finite Element Analysis(FEA) software ANSYS is taken as the simulative tool, 2D simulative model has been set up to investigate the effect of the thickness of coating and/or substrate on the detestability of deboning in MCPs. Two parameters, namely the maximum defect temperature difference ($\Delta T_{D\max}$) and defect appearing index (DAI), are defined to evaluate the detection of defects, and their computational methods and formulas are given respectively. The preliminary changing tendency of $\Delta T_{D\max}$ and DAI with the thickness of coating and/or substrate are found by numerical simulation.

Keywords: *Metallic Composites Plates(MCP); Infrared thermography; NDT(Non-Destructive Testing); Numerical simulation.*

H15

Modeling of Recirculation Zone around the Nozzle Used in Spray Forming

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In spray forming, the flow pattern of atomizing gas plays an important role in the atomization process, especially for a gas recirculation zone located downstream of the delivery tube, which dramatically influences the initial atomization of melt. In this paper, gas-only flow inside and outside the recirculation is analyzed numerically using a commercial computational fluid dynamics (CFD) software Fluent. Analysis on the structure of the recirculation and gas moving inside the recirculation is carried out for various nozzle configurations, protrusion lengths of the melt delivery tube, applied gas pressures and incline angles of the gas nozzle. Meanwhile, the influence of the recirculation on the preliminary disintegration of melt flow is analyzed using CFD. Results show that a turbulent layer separates recirculation zone and high speed gas outside this area. In the center of the recirculation, gas moves towards the melt delivery tube, then encounters gas emitted from the gas nozzle around the stagnation point, where the gas velocity almost drops to zero, but the gas pressure rises. Results also show that the structure of the recirculation is periodic variation, which also implies the atomization is a periodic process.

Keywords: *recirculation, spray forming, gas nozzle, atomization*

H16

Modified QUICK Schemes for 3D Advection-diffusion Equation of Pollutants on Unstructured Grids

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In framework of FVM, two modified QUICK schemes, namely Q-QUICK and UQ-QUICK, for improving the precision of convective flux approximation are verified in 3D unsteady advection-diffusion equation of pollutants on unstructured grids. The constructed auxiliary nodes for Q-QUICK/UQ-QUICK are composed of two neighboring nodes plus the next upwind node, the later node is generated from intersection of the line of current neighboring nodes and their corresponding interfaces. The numerical results show that Q-QUICK and UQ-QUICK have a little higher computational accuracy to CDS and similar numerical stability to UDS/HDS/PDS after applying the deferred correction method. Furthermore, their corresponding CPU times are approximately equivalent to those of traditional difference schemes. In addition, their abilities for adapting high grid deformation are robust. It is so promising to apply the suggested schemes to simulate pollutant transportation on arbitrary natural boundary in hydraulic or environmental engineering.
Keywords: *3D Unstructured Grids, Q-QUICK,UQ-QUICK , 3D Advection-diffusion Equation of Pollutants, FVM*

H17

Mechanism of Re-scaling Frequency Stochastic Resonance Based on Kramers Rate

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We develop and further explore the mechanism of re-scaling frequency stochastic resonance (RFSR) based on the Kramers rate. We find that when the input signal frequency for stochastic resonance (SR) exceeds the half the Kramers rate limit, a frequency-scale ratio of RFSR should be selected to re-scale the larger signal frequency to a small SR frequency. Within the SR frequency range, we compare the performance of two approaches of realizing SR, the method of adjusting system parameters and the method of frequency-scale ratio. We showed that the former makes the half the Kramers rate approaching the signal frequency, while the latter makes the signal frequency approaching the half the Kramers rate. We demonstrate that the method of adjusting system parameters is unable to realize SR under the condition of large signal frequencies. An engineering example demonstrates excellent performance of the re-scaling frequency for SR in fault diagnosis.
Keywords: *Re-scaling Frequency Stochastic Resonance, bistable system, noise, information detection*

H18

Modeling and Simulation for Electromagnetic Shielding Performance of Magnesium

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Magnesium and magnesium alloys are green engineering materials for 21st century. In the paper, we build the model of electromagnetic shielding performance of Magnesium according to different media around Magnesium. If magnesium is plated on engineering plastic board, the simulations show that the ability for magnesium to reflect electric-field component is a little better than the ability for magnesium to reflect magnetic-field component. whether magnesium shielding layer is surrounded with air medium, or magnesium were plated in engineering plastics board, the shielding effectiveness of magnesium varies with thickness of magnesium material and frequency of electromagnetic wave.

Keywords: *Electromagnetic shielding, Magnesium, Modeling, Simulation*

H19

Effects of conformal cooling channel on injection molding and productivity

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In order to prove that the conformal cooling channel is superior to the conventional cooling channel, the three-dimension model of fragrance lamp and two different cooling layouts for the injection mold were carried out using virtual prototypes.

The common defects of injection-molding product such as large warpage, deformation, stress cracks, sink marks, uneven surface gloss and size change are caused mostly by the uneven cooling. In addition, an efficient cooling can reduce the cooling time, which drastically increases the productivity as well as reduce costs, both in lead-time and man-hours.

The traditional cooling channels are based on a conventional machining process such as straight-drilling or groove-milling. For the complicated geometric cavity, it is incapable of fabricating counter-like channels or anything vaguely in three-dimension space. As the mobility of the cooling fluid within the mold is confined, it will cause uneven cooling in the plastic parts.

A proper solution to this problem is performed by the coolant flows in a conformal cooling channel, which is as close as possible to the mold cavity surface to absorb more heat from the molten plastic [1]. Another advantage is that the mold reaches the operation temperature quicker than a conventional one [2,3]. With the development of new rapid tooling techniques such as layered tool construction or metal spray concepts, it is possible to design the conformal cooling channels in an almost unlimited range of shapes[4~7]. The cooling channels can also go around the ejector pins and the feed systems and thus

provide extremely even cooling of the entire mold.

This paper presents an investigation on the two different cooling layouts in an injection mold using the Pro/Engineer and Moldflow software and determining which one offers the most effective heat removal.

The model chosen for the simulation is an injection-molded fragrance lamp designed with Pro/Engineer wildfire 5.0. The virtual models of fragrance lamp and the different cooling layouts were analyzed using Moldflow Plastic Insight 6.1. Parameter inputs are the same for the two different cooling simulations.

The analysis shows that the conformal cooling channel can offer a more uniform heat dissipation, lower volume shrinkage and shorter time to freeze than the conventional channel, which indicates a significantly improving of productivity with expected optimization of the part quality.

The ensuing analysis on this particular plastic part using Moldflow obtains the following results:

(1) 29.7% of maximum cavity surface temperature and 41.2% of average cavity surface temperature can be reduced by applying the conformal cooling channel. It shows that the conformal cooling channel can offer more uniform heat dissipation than the conventional channel, which indicates more accurately control of the temperature of the mold;

(2) 74.0% of maximum differential cooling variation can be reduced by applying the conformal cooling channel. It shows that the conformal cooling channel can offer lower volume shrinkage than the conventional channel, which indicates a significantly improving of the part quality;

(3) 72% of cooling time reduced by applying the conformal cooling channel. It shows that the conformal cooling channel can offer shorter time to freeze than the conventional channel, which indicates a significantly improving of productivity.

This research can be a practical aid in optimizing mold and cooling design. It can also serve as a reference for the comparison of the cooling efficiency and the dimensional accuracy between different layouts. The limitation of the research is that the cooling channel cross section is circle, which is the same with the common characteristic of mechanical processing. The further work required will create innovative cross sections to achieve further improvement of the cooling efficiency.

Keywords: *conformal cooling channel, injection mould, cooling simulation*

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H20

A symmetry-homotopy hybrid algorithm for solving boundary value problem of partial differential equations

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In this paper, we propose a symmetry-homotopy hybrid algorithm to solve boundary value problem of a partial differential equations. We are interesting to consider each other complementariness of both homotopy perturbation method (HPM) and symmetry method to solve boundary value problem of a partial differential equations. In this algorithm, the multi-parameter symmetries of a given partial differential equations provide the reductions of the boundary value problem to a initial value problem of the reduced original differential equation (ODE). The reduction is smaller by properly selection of the symmetry parameters. Then homotopy perturbation method gives the solutions of the initial value problem. Consequently, we solve the boundary value problem by combination of two methods.

h21

A Study of the Measurement Method of Spheroidizing Rate on Coils of Low Carbon Steel

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This paper presents the measurement methods of spheroidizing rate on coil of low carbon steel and the relationship between heat treatment process and spheroidizing rate. The classification of spheroidizing rate is approached by two ways. One is to compare the metallographic with JIS G3539 Standards manually; the other is to calculate the length-width ratio in a SEM metallographic by a computer program which carries on the image recognizing automatically. This method has more efficiency and accuracy than comparing the metallographic with JIS Standards manually. This paper discusses the efficiency and accuracy about the two measurement methods. In the relationship between heat treatment process and spheroidizing rate, the degree of spheroidizing was No.1 by JIS Standards comparing method and the spheroidizing rate was 99.58% by computer program calculation automatically under the tempering process. The AISI 1022 coil was heated from 20℃ to 715℃ for 3 hours, then kept the temperature on 700℃ for 4.5 hours, and cooled the coil to 20℃ finally.
Keywords: *Coil, spheroidizing rate, low carbon steel*

h22

Detection of Surface Defects by the Photothermal Deflection

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The Photothermal Deflection (PTD) technique [1-3] can determine the thermal properties such as thermal conductivity and thermal diffusivity of all types of materials. The PTD technique consists on heating the material surface by a modulated light beam of intensity that generates a refractive index gradient on the fluid surrounding the sample. The exploration of the area heated by a probe laser beam permits to detect any kind of internal and external defects.

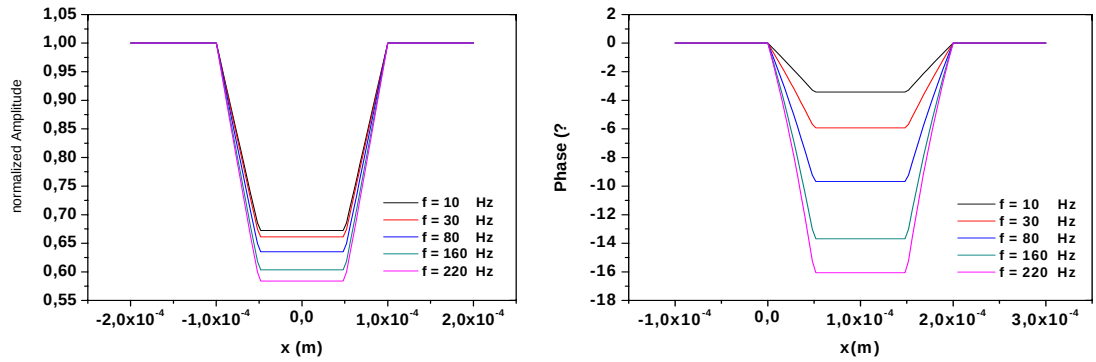
In this paper, we develop a theoretical model which permits to determine the laser probe beam deflection due to variation of the refractive index and to achieve the variations in amplitude and phase throughout a region which is caused a rectangular surface defect. This theoretical study is based on solving the heat equations which brings us the expression of the probe laser beam deflection. In the case of heating by a laser pump beam; the intensity take the following expression and the deflection is the sum of two components; normal deflection and tangential deflection which have respectively the following expressions:

And

$$\psi_n(x,z) = -\frac{1}{n}\frac{\partial n}{\partial T_f}\left[G(0)\sqrt{a^2 - x^2}\,\sigma_f\, e^{-\sigma_f z} + \sum_{n=1}^{\infty} G(n)\frac{\sigma_f(n)}{\alpha_n / a}\cos(\alpha_n x / a)e^{-\sigma_f(n) z}\right]$$

$$\psi_t(x,z) = -\frac{1}{n}\frac{\partial n}{\partial T_f}\sum_{n=1}^{\infty} G(n)\sin(\alpha_n x / a)e^{-\sigma_f(n) z}$$

The distribution of the deflection along the sample surface will give the variation of phase and amplitude versus the defect and the modulation frequency. For a rectangular defect, the following curves show, respectively, the variation of amplitude and phase versus the laser pump beam displacement and for different modulation frequency values.



Keywords: *PTD technique, surface Defects, thermal properties*

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h23

Analysis of Electrochemical Noise and Physical Model of Corrosion Process of Al-Zn-In Series Alloys in NaCl Solutions

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From sacrificial anode materials, Al-Zn-In-Mg-Ti alloys gradually become popular in industry due to their high current efficiency and easy breakdown of the corrosion product, so the alloys are largely used in cathode protection in seawater. In this paper, the corrosion process of Al–5Zn–0.02In–1Mg–0.05Ti (wt %) alloy was investigated by scanning electron microscopy (SEM), energy dispersive X-ray (EDX) and electrochemical noise (EN). The corrosion physics model for describing corrosion process of the alloy in NaCl solutions has been developed. Fig. 1 shows the model including pitting, pitting and dissolution-precipitation and uniform corrosion three corrosion stages. Since the noise data involve information on such stochastic processes as corrosion, they were analysed based upon a stochastic theory: the Weibull probability plot was constructed by fitting Weibull distribution function to the calculated cumulative probability. Based on this, the EN results of every corrosion stages in the model were analyzed using Weibull function. The EDX results show that the alloy is activated by pitting at the initially corrosion stage and by dissolution-precipitation at the later corrosion stage. The above two activation were also confirmed by cumulative probability F (fn) versus the frequency of events fn of shot noise theory. The Weibull probability plots show the three corrosion stages for the alloy. The pitting induction time is longer than that of the dissolution-precipitation, but the activation effect of the dissolution-precipitation is greater than that of the pitting for the alloy.

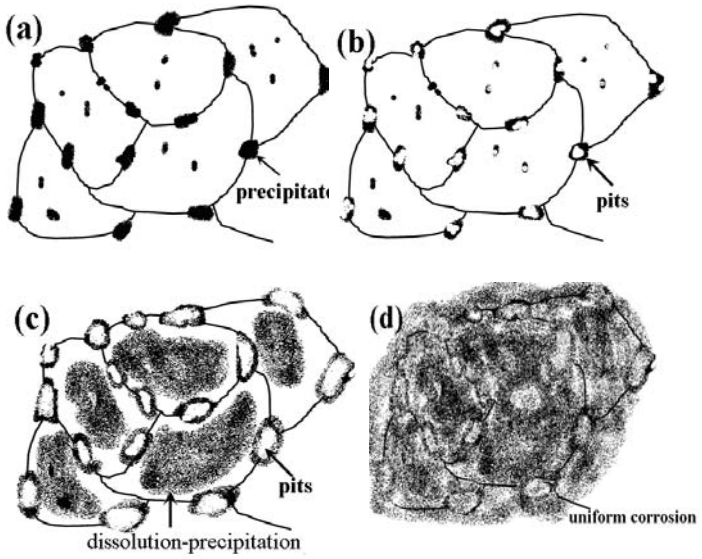

Fig.1 Schematic diagram of corrosion model for Al-5Zn-0.02In-1Mg-0.05Ti alloy: (a) no corrosion; (b) pitting; (c) pitting and dissolved-redeposition; (d) uniform corrosion

Keywords: *sacrificial anode, corrosion, electrochemical noise, Stochastic analysis*

h24

Simulated annealing algorithm and optical thin film

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Annealing is a physical process, in which a solid is heated to high temperature and then cooled sufficiently slowly, takes up the configuration with minimal inner energy. Simulated annealing algorithm is just a mathematic model, which imitates this physical process. Some researchers have developed many formats. One of them called adaptive Simulated Annealing algorithm, which was brought out by Lester Ingber[1]. This algorithm permits an annealing schedule for temperature decreasing exponentially in annealing-time. The introduction of re-annealing also permits adaptation to change sensitivities in the multi-dimensional parameter-space. So it can statically find the best global fit of a nonlinear constrained non-convex cost-function over a D-dimensional space.

On the other hand, optical thin film is very important in many industry. Mathematically, an optical thin film is regard as a homogeneous plane parallel layer of essentially infinite extent, whose thickness is comparable to the wavelength of the incident radiation and which is mainly characterized by refractive index, extinction coefficient and thickness. A multilayer thin film stack is a finite combination of such layers having different film constants. Baumeister first introduced the idea of computational optimization in the design of optical coatings in 1958[2]. Which is to find parameter of thin film system using optimized algorithm by construct an appropriate merit function. Ant to perform the functions for which they were designed, the films must have proper thickness, roughness and other characteristics. These characteristics must often be measured, both during and after fabrication. There are many data processing after the course of measure[3].

In this paper, we will use simulated annealing algorithm to design optical thin film and introduce its application in thin film parameter measure.

Keywords: *simulated annealing algorithm, optical thin film*

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h25

FEM-based thermo-physical process of laser spot heating of sheet metal

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In this paper, a finite element model of laser spot heat flux was built. Then, finite element simulation of laser spot heating on the forming sheet metals was carried out, the transient temperature fields, displacement fields, stress fields and strain fields were investigated. The proposed model can be used to forecast the thermo-physical process of sheet metal of laser spot heating conveniently. The simulated

results show that: (1) There is a good agreement between the finite element simulations based on the proposed model and the experiments. (2) The temperatures of sheet increase with the increase of the laser power and the heating time. The z displacement of forward direction and reverse direction increase when the laser power increases. The deformation time increases when the heating time increases. (3) Radiation of the laser beam yields to a rapid temperature increase at the irradiated surface, which leads to high temperature gradients between the upper surface and the lower surface. The mechanism of laser spot panel heating is the integrated effects of temperature gradient mechanism.

Keywords: *Laser Bending, Sheet Metal, Mechanism, Finite element simulation*

h26

PML condition for the numerical simulation of acoustic wave

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In the numerical simulation of the wave equation, to develop an absorbing boundary condition in the finite domain is a very important problem. Berenger introduced a new condition called the perfectly matched layer, which has the remarkable property of having a zero reflection. Over the last decades, the PML has been used in the context of the acoustic wave equation formulated as a first-order system in velocity and stress, but hasn't been used in the context of numerical schemes that are based on the wave equation written as a second-order system in displacement. The goal of this article is to reformulate PML condition in order to use it in this context.

Keywords: *Acoustic wave equation, absorbing boundary condition, PML, second- order, displacement*

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Development and Modeling of Production Management and Decision Analysis System for Finishing Workshop Based on multi-Agent

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In recent years, with the development of computer, network and communication technology, the information technology was widely used in the textile enterprise, which has efficiently improved production management level [1], and then, many information management systems have been appeared, such as information management system of the textile enterprise, loom monitoring system based on C/S mode, etc. All these systems have successfully applied in the textile enterprise, obtained some good results, realized networking production management from dealing with the internal business to

monitoring and control of the production process [2], and made networking management of the textile enterprise be possible [3]. However, for finishing workshop, there has much more sub-workflow than other workshops, and the different workflows are to be irregularly distributed, which bring the great difficulty to manage production data [4]. As a result, the production management level still stay in the traditional manual management mode, a number of operations, such as computing, statistics and analysis of the various production data, printing all reports, are realized by the manual calculation.

In order to improve the production management level of finishing workshop, to aim at the limitations of the existed information management systems, and the complexity of production management process, first, we analyze the actual requirements and current business management process of the workshop, in the local area network (LAN), use multi-Agent-oriented system design approach [5], and make a new type multi-Agent production management model be designed and realized. Then, the structural model rationality of the system is analyzed, and a collaborative relationship model among multi-Agent is proposed [6]. Third, the core management functions, working principle and message communication flow of multi-Agent is introduced, and the existed production management model is optimized, meanwhile, a flexible, dynamic, efficient collaboration management platform which is for production management and decision analysis is formed. Forth, we analyze and compare several numerical approximation algorithms [7], and put forward a correlation analysis method for production data. Finally, through using network technology, database technology, communication technology and transaction mechanism [8], etc., a multi-Agent production management and decision analysis system is developed for finishing workshop.

As verified by practical application, for finishing workshop, multi-Agent structure model effectively settles the problems that production data is sole and poor sharing, resolves data-processing issues generated by multi-process, multi-variety production management way, and simplifies production management workflow, furthermore, the system functions meet the actual requirements of production management, can accurately deal with production data, timely provide correct production management decision data basis for plant-level managers, and also, in the LAN, multi-Agent production management and decision analysis system boosts information technology development of the textile industry, and provides some technical supports for textile mill to further build the information sharing platform of the business management data.

Keywords: *modeling, multi-Agent, finishing workshop, decision analysis, production management*

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Optimization of Pellet Production Process Parameters in Annular Cooler Using Simulation Results

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A mathematical model of pellet cooling process in annular cooler is established and solved with the commercial software FLUENT in the paper. The model is verified by experiment, and then simulation is conducted. The flow and temperature field are obtained. On the basis of simulation results an orthogonal regression test is performed, the quantitative relations between the cooling effect of annular cooler and the process parameters have been achieved. The effect of process parameters on pellet quality is discussed, the optimized control and operation parameters for pellet cooling is gained. The results are useful to optimizing the pellet cooling process.
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Keywords: *annular cooler, pellet, simulation, orthogonal regression, optimization*

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Performance, Flow and Thermal Characteristics of a Viscous Micro/Nano Pump Simulated by Particle/Continuum Methods

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A novel viscous micro/nano pump consists of a cylindrical rotor eccentrically placed inside a microchannel, where the rotor axis is perpendicular to the channel axis. When the cylinder rotates, a net force is transferred to the fluid because of the unequal shear stresses on the upper and lower surfaces of the rotor. Consequently, this causes the surrounding fluid in the channel to displace toward the microchannel outlet. It is suited for hauling various fluids in microducts. In the case of pumping gas in such small device, the noncontinuum effect will be significant and the operation of the micro/nano viscous pump may not be predicted by continuum assumption-based Navier-Stokes equations. But for liquids in such dimension, the continuum method is still available. The thermal aspect is particularly important for viscous micro/nano pumps due to its large viscous action, small size and the potential application to pump thermosensitive biological fluid.
Based on the Volume-CAD framework [1], two flow solvers have been developed by the authors: one is a particle method, i.e., direct simulation Monte Carlo (DSMC) package V-DSMC; another one is Navier-Stoke solver V-Flow. In this paper, both of the two solvers are used to model the viscous micro/nano pump; V-DSMC is used to model gas flow and V-Flow is applied to the simulation of the pump applied to liquid.

The pumping performances including the pressure drop, flowrate and frictional drag, as well as the flow field characteristics are calculated with the variations of geometrical configurations (eccentricity factor and ratio of channel height to rotor diameter), and compared under different media. In the case of the pump applied to gas, the significant roles of the rotor boundary condition to the performance and flow field characteristics are demonstrated. The thermal effects for different media are also compared; it is not appreciable for gas, but it is significant in the case of liquid, such as glycerin.

Keywords: *micro/nano viscous pump, V-DSMC, V-Flow, pumping performance, flow characteristics, thermal characteristics*

31 May (Monday)

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