Numerical Simulation of Low Pressure Carburizing Incorporating Part Geometry

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Low pressure carburizing is attracting attention as a technology that can reduce CO2 emissions because it uses less hydrocarbon gas than conventional gas carburizing. Industrial parts such as gears have different geometries such as tooth flanks, tooth bottoms, and tooth tips. Since the carbon diffusion field overlaps differently in each area, different carbon concentration profiles can be obtained in each area even with the same carburizing pattern. Therefore, it is of practical importance to estimate an accurate carbon concentration profile for each site for the design of parts such as gears.

It has been reported that the carbon concentration distribution at low pressure carburizing in case-hardening steel can be accurately estimated by the following method. The method is a combination of a local equilibrium calculation that takes into account the existence of two phases, austenite (γ phase) as the matrix phase and cementite (θ phase) as the precipitating phase, and a time evolution calculation of carbon diffusion, assuming that the carbon activity on the steel surface is 1 (a_C=1) as a boundary condition during the carburizing period. This method is a "Model for Diffusion dispersed System". The growth and disappearance of the θ-phase occur in a very small area, less than a few 10 μm from the surface, and high spatial and temporal resolutions are required to reproduce them. In addition, when targeting an object with complex overlapping diffusion fields, such as a gear, the computational domain must be at least two-dimensional, and if high spatial resolution is applied to the entire area, the number of elements becomes enormous, making the method impractical in terms of efficiency and computation time.

In this study, we investigate an efficient method for predicting the distribution of 2-D carbon concentration assuming gears. In order to achieve both accuracy and computation time, we applied hierarchical grid refinement, which increases the resolution of the computational grid only where resolution is necessary, to the numerical calculations and employed parallel computation using GPUs. The calculated and measured values are in good agreement, and it is now possible to efficiently perform carbon concentration distribution not only on the gear tooth surface but also on the tooth tips, tooth bottoms, and other areas with different geometries in this model.

Keywords: *low pressure carburizing, numerical simulation, parts geometry, gpu computing*

1. Introduction

Carbon concentration distribution in low pressure carburizing is accurately predicted by considering boundary conditions where the carbon activity ac of graphite standard is set to 1, performing equilibrium calculations considering coexistence of austenite (denoted as γ) and cementite (denoted as θ), and sequentially conducting time-evolution calculations of carbon[1,2]. However, the growth and decomposition of the θ phase is on the order of tens of seconds and a few micrometers[3], significantly smaller in space and time compared to carbon diffusion in the depth direction (about 1mm in a few hours). Thus, the spatial and temporal resolution of numerical simulations predicting carbon concentration distribution needs to match the growth and decomposition of the θ phase, requiring an order of micrometers and milliseconds. To conduct numerical simulations of carbon concentration distribution reproducing shapes like gears, a 2D area of roughly 8mm square is necessary. Assuming a resolution of 1μm, the element count becomes 64 million elements, making calculations inefficient.
This report introduces cases where 2D carbon concentration distribution numerical simulation in low pressure carburizing were made more efficient without compromising accuracy by utilizing hierarchical direct lattices and symmetrical properties.

2. Numerical Simulation Method

To easily handle diffusion of intrusive atoms like carbon, we use the u-fraction[4]. The relationship between u-fraction u and mass concentration c is expressed in equation (1) as:

$$c = \frac{100u}{\frac{m_\gamma}{m_C} + u} \tag{1}$$

Where m_γ is the molar weight of the γ phase, and m_C is the molar weight of carbon. The time evolution of u is given by equation (2):

$$\frac{\partial u}{\partial t} = \nabla(\lambda M_\gamma y_\gamma \nabla \mu_C) \tag{2}$$

Here, λ depends on the volume ratio of the γ and θ phases and is called the labyrinth factor[5], M_γ is the atomic mobility of carbon in the γ phase, y_γ is the sub-lattice concentration of carbon in the γ phase, and μ_C is the chemical potential of carbon.

In this study, considering the alloy composition of SCr420, $\lambda M_\gamma y_\gamma$ and μ_C were calculated as a function of u-fraction. $\lambda M_\gamma y_\gamma$ and μ_C at 1203 K are shown in Figure 1. The A_{CM} line and the position of u-fraction corresponding to a_C=1 are indicated by dashed lines. Above the A_{CM} line, the mobility term decreases above the A_{CM} line and the potential gradient becomes smaller. This indicates that carbon diffusion is more restricted in the γ + θ 2-phase region than in the γ single-phase region. This approach is referred to as “Diffusion in dispersed systems”[6]. While the only output information obtained is concentration and phase fraction, the input is simple and its versatility is highly regarded.

For the carburization period, a u corresponding to carbon activity a_C=1 was given on the surface, and for the diffusion period, the Neumann boundary condition was applied to simulate low pressure carburizing in a closed system. Calculations for the time evolution of u used the difference method and an explicit method, and the primary calculations were executed through parallel computing with a single GPU. Since the GPU has many cores, it can handle matrix operations at the block level quickly and is compatible with the hierarchical direct lattice we will explain.

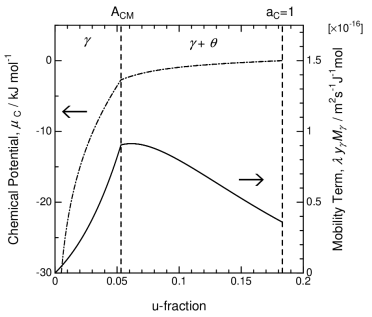

Figure 1 Mobility term and chemical potential of carbon in the γ phase as functions of u-fraction at 1203 K.

The simulation area was created by binarizing a photograph of the cross-section of an actual gear component and extracting the symmetric portion. Figure 2(a) shows the original photograph, while Figure 2(b) illustrates the extracted symmetric portion.

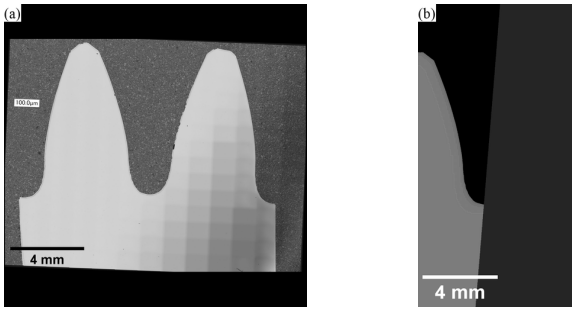

Figure 2 (a) photograph of cross-section of gear component (b) the simulation area was created by binarizing a photograph of the cross-section of an actual gear component and extracting the symmetric portion.

Hierarchical grid refinement: In low pressure carburizing, the surface vicinity (below 0.1mm) sees the growth and decomposition of the θ phase, resulting in steep concentration gradients. In contrast, the concentration gradient of the hardened layer depth (above 0.5mm) is more gradual. Therefore, by subdividing only the surface vicinity where high resolution is needed and lowering the resolution of the remaining parts, the element count can be reduced while maintaining accuracy. As shown in Figure 3(a), a hierarchical direct lattice was used for spatial division. Calculation element sizes, or lattice sizes, were prepared at four levels: 1μm, 2μm, 4μm, and 8μm.

Cyclic or symmetric boundary conditions: The simulation area contains mirror-image objects and periodically repeating target sites, and the number of elements can be reduced by imposing Neumann boundary conditions on the symmetry axes to reproduce symmetry. Figure 3(b) shows the boundary conditions imposed in the simulation area in this study.

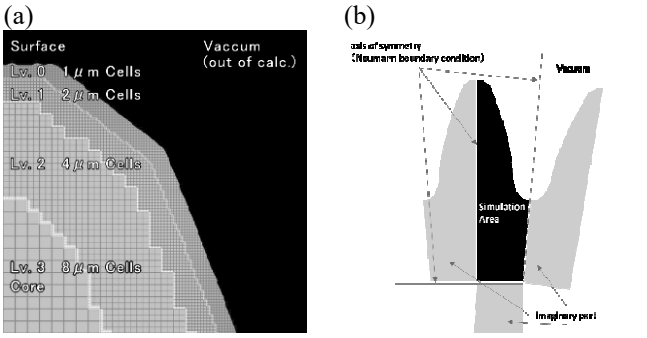

Figure 3 Optimization of the number of elements in the simulation. (a) hierarchical grid refinement. (b) (Cyclic) symmetry boundary conditions used in this model.

The simulation area used in this study is represented by approximately 1.87 million elements, with a minimum element of 1 μm, a short side of 8.192 mm, and a long side of 16.384 mm. This is 3.5% of the number of elements compared to approximately 53.14 million elements without element reduction.

3. Results and Discussion

Numerical simulations of low pressure carburization were performed using the above method to confirm whether the carbon concentration distribution reflected the part geometry. The sample is the gear shown in Figure 4, and the carburizing temperature was set to 1203 K. Experiments were conducted at 1500 s carburizing followed by quenching, and at 1500 s carburizing followed by 4620 s diffusion.

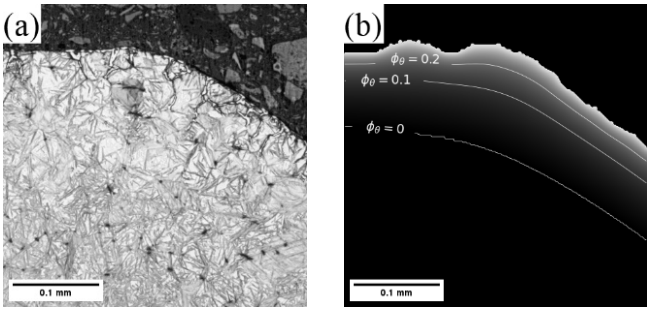

Figure 4 (a) Cross-sectional microstructure of a gear part quenched without diffusion after 1500 s carburizing period. (b) Calculated area fraction of cementite after 1500 s carburizing period at the location corresponding to (a).

Figure 4 shows the simulation and experimental results of the gear top after 1500s carburizing. In the experimental results, white visible grain cementite precipitates along the grain boundary. Although this calculation method does not represent the precipitation of grain boundary carbides, it can be confirmed that the area where cementite is visible in the microstructure photograph is an area where the carbide area fraction φ exceeds 0.1, indicating that the method can

represent carbide precipitation areas several 10 micrometers from the surface.

Figure 5(a) shows a contour plot of the calculated carbon concentration distribution. The white areas show higher carbon concentrations and the dark areas show lower carbon concentrations. The white lines in the figure are the iso-concentration lines at 0.8 wt%, 0.65 wt%, and 0.35 wt%, respectively. Considering the carbon concentration distribution on the tooth surface (PCD) as a reference, the carbon concentration at the tooth top (Top), where the diffusion field overlaps, is higher than that on the tooth surface. On the other hand, the carbon concentration at the tooth bottom (Root), where the diffusion field is sparse, is lower than that at the tooth surface, and the depth of carburization is shallower.

Figure 5(b) compares the measured carbon concentration distribution on the tooth surface (PCD), tooth bottom (Root), and tooth top (Top) of the carburized gear that was actually subjected to low pressure carburizing, analyzed by EPMA, with the calculated carbon concentration distribution at the location corresponding to the actual measurement. The areas where the measurement and analysis were performed are shown in gray in Figure 5(a). The comparison results show that the calculated carbon concentration distribution is in good agreement with the measured distribution. This confirms that the prediction of the carbon concentration distribution is adequate considering the actual gear geometry.

(a) (b)

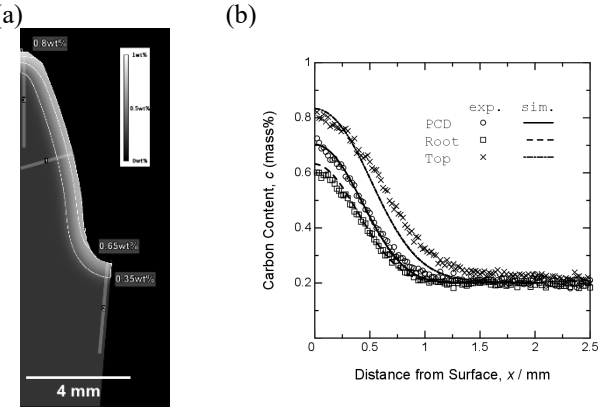

Figure 5 (a) Contour plot of calculated carbon concentration distribution with iso-concentration lines. (b)Calculated carbon concentration distributions at tooth tips, tooth surfaces, and tooth bottoms, and measured values obtained from EPMA analysis of experimentally low pressure carburized gears.

4. Conclusion

A simulation of carbon concentration distribution in low pressure carburizing was performed by incorporating a large-scale numerical method and creating a computational area from an image of an actual part. The numerical results reflect the carbon concentration distribution of the actual part, and it was confirmed that the method can be used to predict the carbon concentration distribution considering the part geometry.

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