Phase-field simulation for the growth of Boride (Fe_2B) phase from Austenite phase

Raden Dadan Ramdan*, Tomohiro Takaki** & Yoshihiro Tomita*
Graduate School of Engineering, Kobe University, 1-1, Rokkodai-chou, Nada, Kobe, 657-8501, Japan
** *Graduate School of Science and Technology, Kyoto Institute of Technology, Sakyo, Kyoto, 606-8585, Japan*

Summary The present paper describes briefly the development of phase-field simulation for the growth of boride (Fe_2B) phase from the austenite phase. In the present work, the problem in defining the free energy of a line compound such as Fe_2B is approached by the assumption that it has a parabolic relationship with the boron concentration. An equilibrium condition can be obtained by one set of free energy applied in the present work. On the other hand, evaluation on the effect of temperature on the growth of boride phase using the present model shows that a higher growth of boride phase was found as the temperature increases from 1193K up to 1273K.

BORONIZING PROCESS

Boronizing is a type of thermo-chemical treatment where boron atom is diffused into the metal substrate during high temperature process to form hard boride structure such as FeB and Fe_2B. Normally it is preferable to have single layer of Fe_2B on the substrate rather than having these two boride phases. The presence of single or mixed layer of boride coating mainly depends on the condition of boronizing process. In most cases FeB phase is considered to form firstly before Fe_2B phase especially for the low temperature process. However, for the case of high temperature process, such as at 950-1100°C and with the longer boronizing time, single Fe_2B boride phase is possible to exist.

Beside having higher hardness compared to other types of thermo-chemical treatment products, boronizing product is also believed to offer a better strength to friction wear and abrasion. Furthermore, its application in industry has been well accepted for long time such as EKabor boronizing agents have proved to be very effective in industrial practice for more than 3 decades. However less study on this process can be found in the literature compared to other types of thermo-chemical treatment. Therefore the present study made an effort to study the growth of single boride phase, Fe_2B, by phase-field method of computer simulation work.

PHASE-FIELD MODEL OF THE GROWTH OF Fe_2B

Phase-field simulation offers a very good explanation on the evolution of one state to other such as in the case of phase transformation. Each state in phase-field model is governed by a number of field variable (Φ). For the present simulation work, Fe_2B phase is set at Φ=1 and austenite phase at Φ=0. The evolution of field variable from 0 to 1 represents the evolution of phase from austenite to Fe_2B or on the other word the growth of Fe_2B phase. In order to perform this simulation work, phase-field model of the boride growth is derived from Ginzburg-Landau free energy functional following the Allen-Cahn equation. This model governs the change of phase-field with time or on the other word the evolution of field variable from austenite to Fe_2B. The model is as follow,

$$\frac{\partial \phi}{\partial t} = M_{\phi}\left\{\varepsilon^2\nabla^2\phi + 4W\phi(1-\phi)\left(-\frac{15}{2W}\phi(1-\phi)\Delta g^{Fe2B,Fe_B^{\gamma}} + \phi - \frac{1}{2}\right)\right\} \cdots\cdots (1)$$

where M_φ is the kinetic parameter related to the mobility of the austenite-boride interface M. W is the potential height and ε_o is the mean value of the gradient coefficient ε_o. On the other hand, Δg is the chemical energy driving force, which is defined as the difference between free energy of Fe_2B and austenite and the set of this energy driving force will be explained subsequently.

Beside the evolution of phase-field model, the model that governs the diffusion of boron or boron concentration profile that accompanies the growth of boride phase is also derived. This model is derived from Ginzburg-Landau free energy functional following the Cahn-Hilliard equation as follow,

$$\frac{\partial X_B}{\partial t} = \nabla\left\{M_B(\phi, X_B, T)\left(\frac{\partial^2 g}{\partial X_B^2}\nabla X_B + \frac{\partial^2 g}{\partial X_B \partial \phi}\nabla\phi\right)\right\} \cdots\cdots (2)$$

where M_B is diffusion coefficient of boron, and is defined as a function of diffusion coefficient of boron in austenite, M_B^{γ}, and boride, M_B^{Fe2B}. Both of these variables were taken from Keddam [1].

FREE ENERGY PROBLEM IN THE PHASE-FIELD SIMULATION OF THE GROWTH OF Fe_2B

One of the big issue in developing the phase-field simulations of the growth of Fe_2B is defining its free energy driving force, since it is a line compound, there is no derivative of its free energy. The common approach to solve this problem is by making an assumption that the free energy of this compound has a parabolic relationship with concentration [2,3,4]. In the present simulation works, 3 sets of free energy were chosen, where the free energy of Fe_2B is fixed and the free energy of austenite is varied at 3 conditions as is shown in the fig.1.

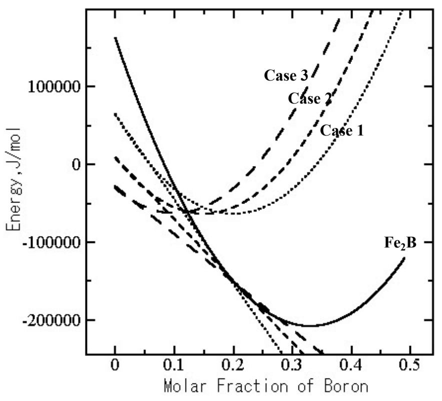
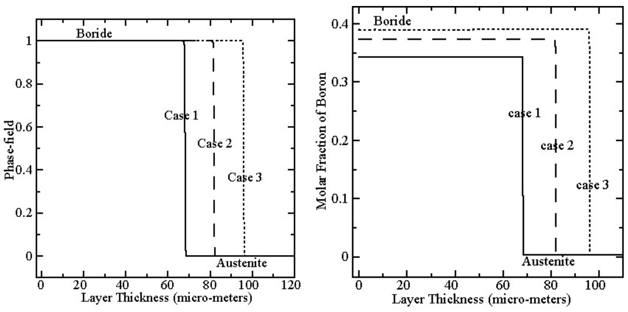


Fig.1 Free energy curve for case 1, 2 and 3 (different set of austenite free energy) and their related common tangent line

RESULTS AND DISCUSSION

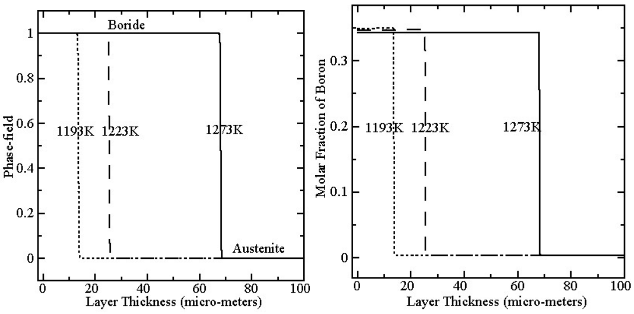
Fig. 2 (a) shows the growth of Fe_2B phase for case 1, 2 and 3. It can be seen from this figure that the growth of Fe_2B phase is higher for the case 3. However according to Fig.2 (b), case 1 is considered to give the more reliable results since the end profile of boron concentration approaching the equilibrium condition for Fe_2B phase which is around 0.33 molar fraction of boron [5].

Using the free energy of the case 1, evaluation on the effect of temperature on the growth of Fe_2B phase was made. Fig.3(a) shows the growth of Fe_2B phase at different temperatures. It can be seen from this figure that the growth of this phase is higher as the temperature increases from 1193K up to 1273K, which is also accompanied with the higher diffusion of boron (Fig.3(b)) for its related temperature. This condition indicates that an effective and efficient increasing of temperature occurs at the chosen range of temperature where a significant increasing of the kinetic of boron diffusion as well as sufficient energy is received by the system for the higher growth of Fe_2B.



(a) (b)

Fig.2 Boride phase growth (a) and boron concentration profile(b) for the case 1,2 and 3



(a) (b)

Fig.3 The influences of temperature on the boride phase growth (a) and boron concentration profile (b)

CONCLUSIONS

One-dimensional phase-field simulation of the growth of Fe_2B phase has been well performed. Three sets of free energy driving force have been determined with the assumption that both free energy of Fe_2B and austenite phase have the parabolic relationship with concentration. An equilibrium condition of Fe_2B phase can be obtained by one set of free energy and evaluation of temperature using this set of free energy indicating a higher Fe_2B phase is growth as temperature increases from 1193K up to 1273K.

References

[1] Keddam. M , A kinetic model for the borided layers by the paste-boriding process, *Applied Surface Science*. **236.** 451–455, 2004

[2] Hu.S.Y *et al.* Thermodynamic description and growth kinetics of stoichiometric precipitates in the phase-field approach. *Computer Coupling of Phase Diagram and Thermochemistry* , **31**. 303-312, 2007

[3] Li., D.Y., Chen, L.Q. Computer simulation of stress-oriented nucleation and growth of θ' precipitates inAl–Cu alloys. *Acta Mater*, **46**, 2573, 1998.

[4] Steibach, I. *et al.* A phase field concept for multiphase systems. *Physica D*, **94**, 135, 1996.

[5] L.G. Yu X.J. Chen K.A. Khor G. Sundararajan, FeB/Fe2B phase transformation during SPS pack-boriding*:* Boride layer growth kinetics, *Acta Materialia* . **53**. 2361–2368, 2005.