Mechanisms of lamellar structure formation and Cr interfacial segregation in C11_b-MoSi₂/C40-NbSi₂ dual phase silicide verified by a phase-field simulation incorporating elastic inhomogeneity

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Abstract

We developed a phase-field model of C11_b-MoSi₂/C40-NbSi₂ duplex silicide incorporating

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elastic inhomogeneity, and simulated microstructure formation and interface segregation. We examined the effect of elastic inhomogeneity on the morphology, volume fraction of the $C11b$ -precipitate, stress distribution, and solute partitioning. In the simulations, parameters evaluated by first-principles calculation are used for the experimentally unknown parameters. The lamellar structure was not formed in the case incorporating the elastic strain energy only and ignoring the anisotropy of the interfacial energy. When the anisotropy of the interfacial energy was taken into account, the lamellar structure was formed parallel to $(0001)_{C40}$ as observed in the experiment. It was also found that the elastic strain energy changes the equilibrium concentrations by > 0.2 at%, but the difference between the equilibrium concentrations in homogeneous and inhomogeneous systems was < 0.1 at%. The interfacial segregation was also hardly affected by the elastic inhomogeneity. These results confirm that elastic inhomogeneity can be neglected in the simulation of $\text{MoSi}_2/\text{NbSi}_2$ lamellar silicide.

Keywords: phase-field simulation; lamellar structure; microstructure; $\text{MoSi}_2/\text{NbSi}_2$

1. Introduction

In order to reduce global warming, a large number of improvements to the refractory materials used for gas-turbine power generation systems are required. Ni-based superalloy is the most representative refractory material, as it is applied in a large number of industrial systems, such as jet engine systems and power generation systems, as materials for turbine blades for instance. This is because this material has beneficial properties such as high-temperature strength, low-temperature toughness, reasonable ductility, oxidation resistance, corrosion resistance and so on. The advantageous mechanical properties are considered to be the result of γ' precipitation in the γ -matrix phase. However, the melting point of Ni-based superalloy is approximately 1,350 °C, and this is not sufficiently high for this substance to be used as a next-generation refractory material. In fact, gas turbines composed of Ni-based superalloy require additional processing including thermal barrier coating and shaping of cooling structure for practical use. Unfortunately however, these additional treatments decreases productivity and thermal efficiency.

As an alternative, MoSi₂-based silicide has been attracting considerable attention as a new high-temperature structural material for use in gas turbine power generation systems. Compared to Ni-based superalloy, MoSi₂ has lower density, a higher-melting point, and good oxidation resistance at even higher temperatures [1-5]. A large number of studies focusing especially on MoSi₂/NbSi₂ alloy have been conducted in the past several decades. In this material, lamellar structures composed of the Nb-rich C40-phase and Mo-rich C11b-phase are formed by directional solidification and heat treatment [6-7]. These lamellar structures play

an important role in providing desirable mechanical properties such as low temperature toughness and high-temperature strength [8-10]. In addition, an MoSi₂/NbSi₂ alloy with Cr doped into the material as an additive element has been shown to be effective as regards the thermal stabilization of a lamellar structure, in comparison with the un-doped counterpart. [11-12]. Further, Cr atoms have been experimentally observed to segregate at the lamellar interface.

The phase-field method is a versatile technique and is widely used for the simulation of microstructural evolution on the basis of thermodynamics and the diffuse interface model. In our previous study, we primarily focused on the segregation mechanism of the additive element. We clarified that the Cr-segregation is largely dependent on the segregation energy, which is the chemical interaction between the solute atoms and the interface which was evaluated by using the first-principles calculation [12-17]. Further, we have examined the dominant factor for the formation of lamellar structure [18]. Generally, the morphology of microstructure consisting of coherent and/or semi-coherent precipitates is determined by the competition between the driving force for reducing elastic strain energy due to coherency strain and that for reducing interfacial energy. We have shown that the formation of MoSi₂/NbSi₂ lamellar structure is dominated by the anisotropy of interfacial energy rather than the elastic strain [18]. However, the calculation of elastic strain energy in the previous study neglected the difference in the elastic moduli between the *C*11_b- and *C*40-phases [18]. Although it is difficult to examine experimentally the effect of elastic inhomogeneity on microstructure formation, it may have a significant impact, and it can be examined by phase field simulation. In fact, it has been reported that a large elastic inhomogeneity can affect

microstructural evolution, yielding a significantly different microstructure to that of an elastically homogeneous system [19-26]. Phase-field simulations of the formation of γ/γ' microstructure in Ni-based superalloy, with the effect of elastic inhomogeneity taken into account, have been already conducted [27, 28], and it was shown that there was little effect of elastic inhomogeneity on the morphology of microstructure formed under no applied stress. However, the microstructural evolution simulated under the condition with external stress and creep strain resembled experimentally observed one more closely when elastic inhomogeneity taken into account than when it was neglected.

The differences in some of elastic constants between $C11_b$ -MoSi₂ and $C40$ -NbSi₂ are larger than those between γ -matrix and γ' -precipitate in Ni-based superalloys while those in others are comparable or smaller. There may be some influences of elastic inhomogeneity on microstructure formation and segregation. It is important to examine whether elastic inhomogeneity significantly affects the morphology of a $C11_b/C40$ lamellar structure. Therefore, here we developed a phase-field model for the MoSi₂/NbSi₂ lamellar structure to verify the dominant factor for the formation of lamellar structure taking into account the effect of elastic inhomogeneity on the morphological evolution of the lamellar structure. We developed the model for elastically inhomogeneous system by modifying the phase-field model for elastically homogeneous system, which was used in our previous study on the segregation mechanism of additive element on lamellar boundaries [13].

In our other previous study on the lamellar structure formation [18], we examined only the qualitative correlation among the morphology, the anisotropy of interfacial energy, and the presence of elastic strain energy. However, it is important to examine the roles of

elastic strain energy more quantitatively for deeper understanding. Therefore, in the present study, we discuss the influence of elastic strain energy for elastically inhomogeneous system in comparison with the elastically homogeneous system from the perspective of energetics. Furthermore, we investigate the effect of elastic inhomogeneity on interfacial segregation and microstructure of solute concentrations.

Thus, the purpose of this study is to examine the effect of elastic inhomogeneity on the microstructural evolution of the lamellar structure utilizing the improved phase-field model for $C11_b$ - MoSi_2 / $C40$ - NbSi_2 alloy system with elastic inhomogeneity.

2. Method

2.1 Model of interface

As mentioned above, the MoSi_2 / NbSi_2 lamellar structure is composed of two phases, i.e., the $C11_b$ - and $C40$ -phase. The lamellar interfaces are formed parallel to the (110) plane of the $C11_b$ -phase and the (0001) plane of the $C40$ -phase with the orientation relationship denoted by $[\bar{1}10]_{C11_b} // [2\bar{1}\bar{1}0]_{C40}$ and $[001]_{C11_b} // [01\bar{1}0]_{C40}$ [7,29]. The atomic arrangements on the planes parallel to the lamellar interface are nearly identical in the two phases as shown in Fig. 1. The (110) plane of the $C11_b$ -structure has ACAC-type stacking, while the (0001) plane of the $C40$ -structure has ABDABD-type stacking. Coherent interfaces can be formed parallel to them, but as is often the case with coherent multiphase alloys, lattice misfit exists across the lamellar interface because of the small but non-negligible differences between the interatomic distances on the planes facing the interface. Several types of lamellar interfaces

with different combination of atomic layers can be formed on the $C11_b/C40$ lamellar interface. The ACACA|BDABDA-type stacking sequence is employed in this study since this type of stacking sequence has the lowest interfacial energy among all the possible types of stacking sequences, as was mentioned in the previous study using the first-principles calculation [17]. Also, both the $C11_b$ tetragonal and $C40$ hexagonal structures have two sublattices composed of transition-metal (Mo, Nb, and Cr) and Si sites. In fact, it is possible for Si atoms to occupy the transition metal sites but, in this study, we ignored Si occupation at those sites as the number of occupying Si atoms is negligibly small. Also, we assumed that the Si atoms are not involved in the phase transformation or solute diffusion of the other elements [30].

The $C11_b$ -MoSi₂ and $C40$ -NbSi₂ pseudo-binary phase diagram, which was produced using the first-principles calculation, shows that the $C11_b$ -phase precipitates from the $C40$ -matrix phase. The order parameter, ϕ , is defined such that $\phi=0$ indicates the $C40$ -phase and $\phi=1$ the $C11_b$ -phase. In the phase-field simulation, the total free energy of the system is described as a functional of the order parameter and solute concentrations, which are functions of position. We take the chemical free energy, the gradient energy, and the elastic strain energy into account as the components of the total free energy, which are expressed as

$$G_{\text{sys}} = \int \left[f_{\text{chem}}(\{c_M\}, \phi) + f_{\text{grad}}(\{c_M\}, \phi) + f_{\text{str}}(\{c_M\}, \phi) \right] dV. \quad (M=\text{Cr, Nb}) \quad (1)$$

Details of each energy component are given below.

3.2 Chemical energy

The chemical free energy density is expressed as,

$$f_{\text{chem}}(\{c_M\}, \phi) = f_{C11_b}(\{c_M\}) \cdot h(\phi) - f_{C40}(\{c_M\})(1 - h(\phi)) + W_{\text{interface}} \cdot g(\phi) + f_{\text{seg}}(c_{\text{Cr}}, \phi) \quad (2)$$

Here, $f_{C11_b}(\{c_M\})$ and $f_{C40}(\{c_M\})$ are the free energy densities of the C11_b and C40 phases, respectively, and these parameters are given as functions of composition using the calculation of phase diagrams (CALPHAD) method [30-32]. W is the magnitude of the energy penalty, which is determined by based on the interfacial energy and the thickness of interfacial region; and $h(\phi)$ and $g(\phi)$ are interpolation functions, given as $h(\phi) = \phi - \frac{\sin(2\pi\phi)}{2\pi}$ and $g(\phi) = \frac{1 - \cos(2\pi\phi)}{2}$. They are different from the commonly used polynomial functions but have the characteristics required for interpolation functions. That is, $h(\phi)$ increases monotonically from 0 to 1 with increasing ϕ increases from 0 to 1, and it satisfies the conditions of $h(0) = h(1) = 1$ and $(dh/d\phi)_{\phi=0} = (dh/d\phi)_{\phi=1} = 0$. The $g(\phi)$ has a double-well type profile with respect to ϕ and satisfies $g(0) = g(1) = 0$ and $g(1/2) = 1$. Finally, $f_{\text{seg}}(c_{\text{Cr}}, \phi)$ is the segregation energy function, which represents the chemical energy due to the interaction between the additive Cr atoms and the atomic layers is the diffuse interface. The details of the segregation energy function was described in the previous paper [13]. Here, the only the essentials of the segregation energy is described. The energies of Cr atoms substituting transition metal sites on atomic layers within the interface region were evaluated by using the first-principles calculation [17]. In order to take this segregation energy into account as a component of the chemical energy, we defined the continuous function as

$$f_{\text{seg}}(c_{\text{Cr}}, \phi) = c_{\text{Cr}} \left\{ \begin{aligned} &\Delta e_{\phi=0.2} \exp\left\{\frac{-(\phi-0.2)^2}{b}\right\} + \Delta e_{\phi=0.4} \exp\left\{\frac{-(\phi-0.4)^2}{b}\right\} \\ &+ \Delta e_{\phi=0.6} \exp\left\{\frac{-(\phi-0.6)^2}{b}\right\} + \Delta e_{\phi=0.8} \exp\left\{\frac{-(\phi-0.8)^2}{b}\right\} \\ &+ \Delta e_{\phi=1.0} \left\{\frac{1-\cos(\pi\phi)}{2}\right\} \end{aligned} \right\}. \quad (3)$$

where $\Delta e_{\phi=p}$'s ($p = 0.2, 0.4, 0.6, 0.8, 1.0$) are the parameters determined from the energies of Cr atoms on the atomic layers whose positions are represented by the value of ϕ within the diffuse interface region, and b is a constant that determines the spread of the Gaussian functions. Gaussian functions are used to interpolate the energies of Cr atoms on the atomic plane to the position between the atomic layers smoothly. In our previous study, it was clarified that the Cr segregation at the lamellar interface was found to be the segregation energy rather than the relaxation of the lattice misfit [13].

2.3 Calculation of elastic strain energy

In order to evaluate the lattice misfit between the $C11_b$ - and $C40$ -phase, the lattice parameters of the two phases are needed to be described as function of ϕ and solute concentrations. The lattice parameters of stoichiometric disilicides of Mo, Nb and Cr for both $C11_b$ - and $C40$ structures were determined using the first-principles calculation. The calculated lattice parameters of experimentally available disilicides have good correspondence to experimental values. We also use calculated lattice parameters of fictitious disilicides such as the $C11_b$ structure of NbSi_2 . This allows us to evaluate the lattice sizes not only as a function of concentration but also as a function of order parameter. By assuming the modified Vegard's law in which the sizes of corresponding lattice are linear function of order

parameter and concentration of transition metal element, the lattice mismatch, η_{ij}^M , is defined using the lattice sizes as

$$\eta_{ij}^M = \begin{cases} \frac{l_{i,MSi_2}^{C11b} - l_{i,MSi_2}^{C40} - (l_{i,MoSi_2}^{C11b} - l_{i,MoSi_2}^{C40})}{l_{i,MSi_2}^{C40}} & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} \quad (4)$$

where l_{i,MSi_2}^{C11b} , l_{i,MSi_2}^{C40} are the sizes of equivalent lattices of $C11b$ structure and $C40$ structure respectively for MSi_2 disilicides of transition metal element M (i.e. $MoSi_2$, $NbSi_2$, $CrSi_2$). The values of the lattice sizes can be found in the previous paper [13]. The directions of coordinate used for the simulation space were defined as Direction 1 $//[110]_{C11b} // [0001]_{C40}$, Direction 2 $//[\bar{1}10]_{C11b} // [2\bar{1}\bar{1}0]_{C40}$, and Direction 3 $//[001]_{C11b} // [01\bar{1}0]_{C40}$. Using the lattice mismatch, the eigen strain, $\varepsilon_{ij}^{\text{eigen}}$, is described as

$$\varepsilon_{ij}^{\text{eigen}}(\mathbf{r}, t) = \eta_{ij}^M (c_M \phi - \overline{c_M \phi}). \quad (5)$$

The inhomogeneous strain, e_{ij}^c , can be expressed as

$$e_{ij}^c(\mathbf{r}, t) = \frac{1}{2} \left(\frac{\partial \mathbf{u}_j}{\partial x_i} + \frac{\partial \mathbf{u}_i}{\partial x_j} \right), \quad (6)$$

where $\mathbf{u}$ is the local displacement vector. The elastic strain, $\varepsilon_{ij}^{\text{el}}$, is expressed as

$$\varepsilon_{ij}^{\text{el}}(\mathbf{r}, t) = e_{ij}^c(\mathbf{r}, t) - \varepsilon_{ij}^0(\mathbf{r}, t), \quad (7)$$

while the elastic strain energy, E_{str} , is evaluated from these equations, such that

$$E_{\text{str}}(c_{\text{Nb}}, c_{\text{Cr}}, \phi) = \frac{1}{2} \int C_{ijkl} \varepsilon_{ij}^{\text{el}} \varepsilon_{kl}^{\text{el}} dV. \quad (8)$$

2.4. Elastic inhomogeneity

The elastic strain, which accommodates the misfit in crystal lattices to allow the formation of a coherent interface, is a significant factor in the formation of the microstructure. Some methods have been proposed and applied to examine conditions in which elastic inhomogeneity is considered [20,23]. Although a large difference in morphology can be found when the inhomogeneous degree of the elastic modulus is larger than 50 % [20], the inhomogeneous effect of the elastic modulus should be assessed in order to evaluate the lattice misfit exactly. In this study, an iterative method is used, since the elastic inhomogeneity of our system is relatively small.

The displacement vector is solved in Fourier space. In the iterative method, we can obtain the first-order inhomogeneous strain, where $e_{kl}^{c[0]}(\mathbf{r})$ is the zero-th order approximation, i.e., we assume elastic homogeneity. Hence,

$$e_{kl}^{c[i]}(\mathbf{r}) = \frac{1}{2} \int_{\mathbf{k}} \left\{ n_k \Omega_{pl}(\mathbf{n}) + n_l \Omega_{pk}(\mathbf{n}) \right\} n_q \sum_M \left\{ \begin{aligned} & C_{pqmn}^M \eta_{mn}^M - \Delta C_{ijkl} \bar{\varepsilon}_{mn}^c \left\{ \phi(\mathbf{r}) c_M(\mathbf{r}) \right\}_{\mathbf{k}} \\ & + \Delta C_{ijkl} \eta_{mn}^M \left\{ \phi(\mathbf{r}) c_M(\mathbf{r}) \right\}_{\mathbf{k}}^2 \\ & - \Delta C_{ijkl} \eta_{mn}^M \left\{ e_{kl}^{c[i-1]}(\mathbf{r}) \phi(\mathbf{r}) c_M(\mathbf{r}) \right\}_{\mathbf{k}} \end{aligned} \right\} \exp(i\mathbf{k}\mathbf{r}) \frac{d\mathbf{k}}{(2\pi)^3} \quad (9)$$

Using almost the same approach as for the first-order calculation, we can obtain the i th result for the inhomogeneous strain, such that

$$e_{kl}^{c[i]}(\mathbf{r}) = \frac{1}{2} \int_{\mathbf{k}} \left\{ n_k \Omega_{pl}(\mathbf{n}) + n_l \Omega_{pk}(\mathbf{n}) \right\} n_q \sum_M \left\{ \begin{aligned} & C_{pqmn}^M \eta_{mn}^M - \Delta C_{ijkl} \bar{\varepsilon}_{mn}^c \left\{ \phi(\mathbf{r}) c_M(\mathbf{r}) \right\}_{\mathbf{k}} \\ & + \Delta C_{ijkl} \eta_{mn}^M \left\{ \phi(\mathbf{r}) c_M(\mathbf{r}) \right\}_{\mathbf{k}}^2 \\ & - \Delta C_{ijkl} \eta_{mn}^M \left\{ e_{kl}^{c[i-1]}(\mathbf{r}) \phi(\mathbf{r}) c_M(\mathbf{r}) \right\}_{\mathbf{k}} \end{aligned} \right\} \exp(i\mathbf{k}\mathbf{r}) \frac{d\mathbf{k}}{(2\pi)^3} \quad (10)$$

where C_{ijkl}^M is the elastic moduli of the $C40$ -matrix phase, ΔC_{ijkl} is the differences of elastic moduli of $C11_b$ precipitate phase (C_{ijkl}^P) from those of $C40$ -phase (i.e. $\Delta C_{ijkl} = C_{ijkl}^P - C_{ijkl}^M$), and $\bar{\varepsilon}_{mn}^c$ is $\overline{\phi(\mathbf{r}) c_M(\mathbf{r})}$. The elastic moduli are set as in Table 1, the parameters of which are

evaluated experimentally [35]. The calculations are conducted for the cases with various iteration numbers of 1, 3, and 5.

Other parameters used in this study are listed in Table 2.

2.5. Interfacial energy anisotropy

The gradient energy, $f_{\text{grad}}(\{\nabla c_M\}, \nabla \phi)$, which is due to the non-uniformity of the order parameter and of the element concentrations in the system, and which is identical to the excess energy at the interface, is expressed as

$$f_{\text{grad}}(\{\nabla c_M\}, \nabla \phi) = \sum_M \kappa_M (\nabla c_M)^2 + \kappa_\phi (\nabla \phi)^2, \quad (11)$$

where κ_M is the gradient energy coefficients for concentrations of solute M ($M=\text{Nb Cr}$), and κ_ϕ is for order parameters which is dependent on the interfacial energy and the interfacial thickness. It has been demonstrated that the $C11_b/C40$ interfacial energy has an extremely large anisotropy by first-principles calculation. The lamellar interface, which has the ACACA|BDABDA stacking sequence, has the lowest energy of $\gamma_{11} = 27.2 \text{ mJ/m}^2$, whereas the interfacial energies on the $(\bar{1}\bar{2}\bar{1}0)_{C40}/(\bar{1}\bar{1}0)_{C11_b}$ and $(10\bar{1}0)_{C40}/(001)_{C11_b}$ interfaces, which are perpendicular to the lamellar interfaces, have very high interfacial energy of $\gamma_{22} = 1762 \text{ mJ/m}^2$ and $\gamma_{33} = 1730 \text{ mJ/m}^2$, respectively. In order to take the anisotropy of the interfacial energy into account, the gradient coefficients of k_{22} and k_{33} are set to be

$$\kappa_{22} = \frac{1762}{27.2} \kappa_{11} \text{ and } \kappa_{33} = \frac{1730}{27.2} \kappa_{11}.$$

2.6. Temporal evolution

The morphological evolution of the $C11_b$ -phase is obtained by solving the Cahn-Hilliard equation [35] for the solute concentrations, and the Allen-Cahn equation [36] for order parameters. These equations are respectively expressed as

$$\frac{\partial c_M}{\partial t} = \left[\frac{D_M c_M}{kT} \left\{ (1 - c_M) \nabla \left(\frac{\delta G_{\text{sys}}}{\delta c_M} \right) - \sum_{M' \neq M} c_{M'} \nabla \left(\frac{\delta G_{\text{sys}}}{\delta c_{M'}} \right) \right\} \right] \quad (M, M' = \text{Cr, Nb}), \quad (12)$$

$$\frac{\partial \phi}{\partial t} = -\alpha \left(\frac{\delta G_{\text{sys}}}{\delta \phi} \right), \quad (13)$$

where D_M is the self-diffusion coefficient of element M and α is the mobility coefficient for the transformation between the $C40$ - and $C11_b$ -phases. The diffusion coefficient terms of M are assumed to be same as that for Mo self-diffusion along the a -axis in $C11_b$ - MoSi_2 obtained experimentally [37]. We employed a relatively low value for α which in order to avoid the $C11_b/C40$ interface migration without being associated with solute diffusion.

2.7. Three-dimensional simulation of microstructure formation

In order to examine the effect of elastic inhomogeneity and anisotropy of interfacial energy on the microstructure. The temporal change of the shape of $C11_b$ precipitate, which is sphere with diameter of $100 \mu\text{m}$ in the initial condition, was simulated under various conditions. Coarse-grained phase-field simulations were conducted for a space with dimensions of $128 \times 128 \times 128 \mu\text{m}^3$, using $128 \times 128 \times 128$ grid points. The alloy composition was $(\text{Mo}_{0.968}\text{Nb}_{0.032})_{0.97}\text{Cr}_{0.03}\text{Si}_2$, and the temperature was 1673 K, which are same as in the experiment to which the simulation result is compared. The thickness of the interfacial region was assumed to be $13 \mu\text{m}$, and a periodic boundary condition was

employed to solve the kinetic equations. As the initial condition, the $C11_b$ -phase with equilibrium concentration was set inside the $C40$ -matrix phase and the concentration and order parameter were allowed to evolve. Then, we examined the effect of the elastic inhomogeneity on the microstructural evolution.

2.8. One-dimensional simulation of interfacial segregation

One-dimensional simulation of interfacial segregation of Cr has been also conducted under the conditions essentially same as in the previous study, except that the elastic inhomogeneity was included in this study while neglected in the previous study. That is, the simulation was conducted for one-dimensional space 12 nm in length using 128 grid points. Composition and temperature selected were also same as in the 3D simulation and in the previous study as well.

3. Result

3.1. Convergence efficiency in relation to iteration number

We aimed to examine the effect of elastic inhomogeneity on this material's microstructure, since the iterative method was employed to determine the constrained stress, as expressed in Eq. (10). We examined the convergence of the microstructure by comparing the stress components while changing the iteration number. From the initial condition of the $C11_b$ -precipitate phase embedded in the $C40$ -matrix phase, we varied the iteration number from 1 to 5, and examined the stress components. These components were evaluated using different iteration numbers and in comparison with the stresses of the elastic homogeneous

system. Fig. 2 shows the distributions of the σ_{22} (Fig. 2a) and σ_{33} (Fig. 2b) stress components, which were parallel to lamellar interface, and which were obtained from the constrained stress by using the iterative method as a function of position for different iteration numbers. The results for the elastically homogeneous system (i.e., the zero-th order approximation) are represented by the solid blue points, while the results for the elastically inhomogeneous system are indicated by the orange cross, the red squares and the black points for different iteration numbers. The stress difference between the zero-th order approximation (i.e. elastically homogeneous system) and the results for the elastically inhomogeneous system obtained using the iterative method can be clearly observed to be approximately 0.5–10 %. For the elastic inhomogeneous calculations, the changes in response to varying iteration numbers is much smaller, as can be seen in the stress profiles. Thus, relatively small number of iteration is required for obtaining sufficiently converged elastic solution for the $C11_b$ - MoSi_2 / $C40$ - NbSi_2 duplex phase system with the elastic moduli shown in Table 1. The ratio of elastic moduli for $C40$ - and $C11_b$ -phase are $\frac{C_{11}^{C11_b}}{C_{11}^{C40}} = 0.99$, $\frac{C_{22}^{C11_b}}{C_{22}^{C40}} = 1.22$, and $\frac{C_{33}^{C11_b}}{C_{33}^{C40}} = 1.35$. The ratio value is 1.35 at most, which is relatively small compared to those for the system with high elastic inhomogeneity, such as metal-ceramics system. Thus, small iteration numbers are sufficient to solve problems involving elastic inhomogeneity for this alloy system.

3.2. Dependence of $C11_b$ precipitate morphology on elastic inhomogeneity

In the previous section, we examined the effect of iteration number for on the

elastic conversion by evaluating the stress distribution in a static system (i.e. without time evolution), and found iteration number of 5 is sufficient to converge stress distribution in the elastically inhomogeneous. Based on the results we chose the iteration number of 5 for further study of temporal evolution of microstructure. The temporal changes in the shape of C11_b precipitate embedded, in the C40-matrix phase driven by the reduction of elastic energy were simulated. In the case of an elastically inhomogeneous system, the precipitation shape is then examined during the resultant growth by comparison with that of the elastically homogeneous system. Here, the shape of the C11_b-precipitate phase developed from a sphere with uniform concentrations of $c_{Nb} = 4.5\%$, $c_{Si} = 66.6\%$, and $c_{Cr} = 1.0\%$, which are also the same in the matrix phase. The volume fraction of the spherical C11_b precipitate was 25 %. Simulations were conducted for three systems: (I) incorporating both elastic inhomogeneity and the anisotropy of interfacial energy, (II) incorporating the anisotropy of interfacial energy while neglecting elastic inhomogeneity, (III) neglecting both the elastic inhomogeneity and the anisotropy of the interfacial energy. The isotropic interfacial energy calculation was conducted assuming $\gamma_{11} = \gamma_{22} = \gamma_{33} = 27.2 \text{ mJ/m}^2$ to reduce the computational cost.

Fig. 3a,b shows the snapshots showing the shape of C11_b precipitate by the distribution of the order parameter at the time steps of 50,000 during the course of temporal evolution towards equilibrium for each system. A distinct difference between the morphology of the elastically inhomogeneous and elastically homogeneous systems is not observed. Fig. 4, where the volume fraction of the C11_b-phase is plotted as a function of the time step and obtained for each simulation condition, shows that there is also very little difference between

the elastically homogeneous and elastically inhomogeneous systems as regards changes in volume fraction. On the other hand, it is clear that the precipitate morphology is significantly different when the anisotropy of the interfacial energy is ignored. In this case, the $C11_b$ -precipitate phase changes its microstructure, having habit planes approximately parallel to $(01\bar{1}0)_{C40}$, $(2\bar{1}\bar{1}0)_{C40}$, $(0001)_{C40}$, $\{10\bar{1}1\}_{C40}$, $\{1y(1+y)0\}_{C40}$, $\{2\bar{1}\bar{1}x\}_{C40}$ (x and y are real numbers), as shown in Fig. 3c; the lamellar structure does not elongate in the direction perpendicular to $[0001]_{C40}$ as in the two other simulations. These simulations suggest that the elastic strain energy does not determine the morphology of the lamellae in this material, regardless of whether the system is elastically inhomogeneous or homogeneous, and that the anisotropy of the interfacial energy determines the formation of the lamellar structure. The elastic inhomogeneity has little influence on the morphology of the $C11_b$ -precipitation phase.

Furthermore, we examined whether the solute concentration distributions can be affected by the elastic inhomogeneity. Fig. 5a shows the calculated Nb distribution at the 50,000 time step. In order to identify the effect of the elastic inhomogeneity, the simulation results for both elastic homogeneity and inhomogeneity are shown for comparison. The numbers in the legend indicate the iteration number used to calculate the elastically inhomogeneous strain. The Nb concentration is partitioned between the $C11_b$ -phase and the $C40$ -phase, and this is in good agreement with the experimental results, but there exist some differences among the distributions of each phase. Fig. 5b,c show the calculated distribution of the stress components for each simulation condition, and a difference also exists between each simulation result. We can identify some differences in the solute concentration regarding

the elastic inhomogeneous strain energy and iteration number required for convergence. Large iteration numbers are not required for the stress to converge from the initial sphere-shape condition, as shown in Fig 5b,c but, as the simulation proceeds, some calculated parameters affect the microstructural evolution depending on the specific simulation conditions.

4. Discussion

The Nb-concentration is found to be influenced by the elastic inhomogeneity as demonstrated in Fig. 5a. Here, we understand the changes in equilibrium concentration of Nb due to the elastic inhomogeneity quantitatively by evaluating the difference in the free energies of constituent phases for the cases with and without elastic inhomogeneity. Fig. 6 shows the free energies of the $C11_b$ - and $C40$ -phases as a function of Nb-concentration (ranging from 0 to 10 at%), for the initial stage of the microstructural evolution. The red and green curves represent the energies of the $C11_b$ - and $C40$ -phases, respectively. The solid curves show only chemical energy, while the dotted curves indicate the sum of the chemical and elastic strain energy for the elastically homogenous system. Similarly, the dashed lines represent the sum of the chemical and elastic energies for the elastically inhomogeneous system.

First, we compare the effect of the elastic strain energy, as shown in Fig. 7. It can be seen that the free energy increases by approximately 220 J/mol when elastically homogeneous energy is considered along with the chemical energy. From this free energy function, we can detect a difference of approximately 0.005 to 0.1 at% in the equilibrium

concentration estimated by the common tangent line of both free energy profiles. On the other hand, little difference can be observed if the energy is considered to be elastically inhomogeneous, as shown in Fig. 8. Similarly, the difference in the equilibrium concentration for each simulation condition can be observed to be approximately 0.02 to 0.05 at% at most.

Finally, we examined the effect of the elastic inhomogeneity on the Cr-segregation, which was observed experimentally by our co-researcher [11,12]. In our previous research, we developed a simulation model for Cr-segregation at the C11_b/C40 lamellar interface. It was difficult to observe segregation forming at the small layer since we employed a coarse-grained phase-field model. Another simulation was conducted for a 12-nm-long dimensional space using 128 grid points, which considered the actual interfacial width in order to allow the Cr atoms to segregate at the interface. Using this simulation model, Cr-segregation of 1.754 at% was identified in our previous research, where elastic homogeneity was considered for the elastic strain energy, as shown in Fig. 9. If we ignore the elastic strain energy, i.e., if only the chemical energy is considered to be the driving force of the microstructural development, a difference of 0.03 at% is observed, compared to the simulation condition in which the elastic strain energy is also taken into account. On the other hand, the difference is 0.003 at% at most if elastic inhomogeneity is incorporated into the simulation system. Therefore, the elastic strain energy can play an important role in the equilibrium concentration, since it has the potential to change the segregation amount by as much as several percent, but the elastic inhomogeneity does not make a significant difference to the equilibrium concentration of each phase and to the level of segregation. From the above, the elastic inhomogeneity has little influence on the microstructural formation or

element concentration distribution in $C11b/C40$ lamellar silicide, although it can affect the results of our previous calculations, in which elastic homogeneity was assumed.

5. Conclusions

We developed a phase-field model incorporating elastic inhomogeneity and, using this model, examined the effect of this inhomogeneity on the morphology of $\text{MoSi}_2/\text{NbSi}_2$ lamellar silicide. This was done by comparing the simulation results for the elastically inhomogeneous system to those for the elastically homogeneous system. In both cases, the initially sphere-shaped precipitate changed to a plate-shaped one to form a lamella. However, we did not observe a distinct morphological difference between the results of the elastically inhomogeneous and homogeneous systems; further, there was little difference in the distribution of the concentration and stress. On the other hand, in the case where the anisotropy of the interfacial energy was not considered, we observed a microstructure with habit planes parallel to $(01\bar{1}0)_{C40}$, $(2\bar{1}\bar{1}0)_{C40}$, $(0001)_{C40}$, $\{10\bar{1}1\}_{C40}$, $\{1y(\overline{1+y})0\}_{C40}$, $\{2\bar{1}\bar{1}x\}_{C40}$ planes instead of lamellae. These results suggest that the anisotropy of the interfacial energy, rather than the elastic strain energy, is responsible for the lamellar structures in $\text{MoSi}_2/\text{NbSi}_2$. In order to interpret the change in solute concentration due to elastic strain energy quantitatively, we evaluated the equilibrium concentrations from the calculated free energy curves for the cases with and without elastic energy included. The effect of the inclusion of the elastic strain energy could be clearly observed since the free energy increased, but the addition of elastic inhomogeneity had little influence on the free

energy and equilibrium concentration. The results of this study is important as a basis for conducting further study of microstructural evolution in the $\text{MoSi}_2/\text{NbSi}_2$ based alloys with other alloying elements, which will be presented in the near future. The finding of the negligibly small influence of elastic inhomogeneity allowed us to conduct the simulations neglecting the elastic inhomogeneity with is significantly less inexpensive computationally than those taking into the elastic inhomogeneity.

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Captions

Table 1. Elastic modulus for each tensor in $C11_b$ and $C40$ -phase [33, 34].

Table 2. Parameters used in the simulations.

Fig. 1. Unit cells of (a) $C11_b$ -structure and (b) $C40$ -structure. Large balls show transition metals (Mo or Nb atoms) and small ones show Si atoms. Atomic arrangements on (c) (110)-plane of $C11_b$ -phase and (d) (0001)-plane of $C40$ -phase, which are parallel to the $C11_b/C40$ lamellar interface.

Fig. 2. Distribution of the stress component (a) σ_{22} and (b) σ_{33} along Direction 1 across $C11_b$ -precipitate under the initial condition. Blue points indicate the results obtained for elastically homogeneous system, and yellow, red and black markers show those for elastic inhomogeneous system and iterative method with number of iterations of 1, 3, and 10 respectively. Numbers after markers indicates iteration number. The value of stress is given in non-dimensional unit reduced by RT/V_m , where R is the gas constant, T the absolute temperature, and V_m the molar volume.

Fig. 3. Distribution of the order parameter of cross section obtained under different simulation conditions: (a) elastically homogeneous system with anisotropic interfacial energy, (b) elastically inhomogeneous system with anisotropic interfacial energy, and (c) elastically homogeneous system with isotropic interfacial energy.

Fig. 4. Distribution of volume fraction of $C11_b$ -phase obtained by two simulation conditions. Red line shows the result of elastic homogeneity and blue line shows that of elastic inhomogeneity.

Fig. 5. (a) Nb-concentration and (b, c) stress distributions along center line of the simulation space obtained for different elastic condition at the same time step of 50,000. Number of iterations for calculating elastic inhomogeneity are 3 and 5. The value of stress is given in

non-dimensional unit reduced by RT/V_m , where R is the gas constant, T the absolute temperature, and V_m the molar volume.

Fig. 6. Gibbs free energies of $C11_b$ -phase and $C40$ -phase at 1673 K as a function of Nb concentration. Solid lines, dotted lines and dashed lines show summation to chemical energy.

Fig. 7. Comparison of Gibbs free energies between chemical energy (solid line) and chemical energy plus elastic homogeneous energy (dotted line).

Fig. 8. Comparison of Gibbs free energies between chemical energy plus elastic homogeneous energy (dotted line) and chemical energy plus elastic inhomogeneous energy (dashed line).

Fig. 9. Profiles of Cr-concentration obtained after equilibration in one dimensional simulation conducted under different elastic conditions. Each arrow shows amount of Cr-segregation at the interface.

Table 1. Elastic constants of $C11_b$ -phase and $C40$ -phase [31, 32].

	C_{ij} [GPa]								
	C_{11}	C_{22}	C_{33}	C_{12}	C_{13}	C_{23}	C_{44}	C_{55}	C_{66}
$C40$	380	380	468	152	89	89	145	145	76
$C11_b$	417	417	515	104	84	84	204	204	194

Table 2. Parameters used in the simulations.

Physical properties	Value [unit]
self-diffusion coefficient: D_0	1.4×10^{-3} [m ² /s]
Activation energy: Q	468 [kJ/mol]
Temperature: T	1673 [K]
Diffusion coefficient: D_M	3.4×10^{-18} [m ² /s]
Mobility for order parameter : α	2.0×10^{-16} [m ³ /(J·s)]
Interfacial thickness: 2λ	13 [μm]
Gradient coefficient: κ	2.7×10^{-4} [J/m]

Fig. 1. Unit cells of (a) $C11_b$ -structure and (b) $C40$ -structure. Large balls show transition metals (Mo or Nb atoms) and small ones show Si atoms. Atomic arrangements on (c) (110) -plane of $C11_b$ -phase and (d) (0001) -plane of $C40$ -phase, which are parallel to the $C11_b/C40$ lamellar interface.

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Graphical Abstract