Multiscale Approach for the Deformation Mechanism in Pearlite Microstructure

Atomistic study of the role of the heterointerface on ductility

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Abstract

The role of the ferrite/cementite heterointerface on the mechanical properties of heavily-drawn-pearlitic steel is investigated via tensile deformation tests of multilayered composite models with brittle and ductile virtual materials in a two-dimensional triangle-lattice system by using molecular dynamics simulations. The interface strength is controlled by introducing a heterointerface potential. The dominant role of heterointerface on the mechanical properties of multilayered composite models is influenced by the interface strength. In case of weak interface strength, the heterointerface acts as a strong barrier to dislocation motion in the ductile phase; hence, the multilayered composite model shows high strength but extremely low ductility. This tendency corresponds well to that of as-drawn pearlitic steel with cementite decomposition. In case of strong interface strength, the heterointerface acts as a dislocation source of the brittle phase by dislocation transmission through the heterointerface from the ductile to brittle phase; hence, the multilayered composite model shows good ductility with a small decrease in strength. This tendency corresponds well to annealed pearlitic steel recovered from cementite decomposition. These results suggest that cementite decomposition decreases the plastic deformation potential of the heterointerface. The conditions necessary for the heterointerface to simultaneously exhibit high strength and ductility are discussed on the basis of the results of atomic simulations.

Keyword: Pearlitic steel, Heterointerface, Atomic simulation, Mechanical property, Ductility, Cementite decomposition

1. Introduction

Pearlitic steel is a widely used material in industry [1,2]; its characteristics are attractive because it exhibits high strength and ductility after line-drawing and annealing processes [3]. The microstructure of pearlite is composed of lamellae of ferrite and cementite phases oriented parallel to the drawing direction [4]. This orientation means that under a constant strain condition, the cementite phase in pearlite microstructure must receive almost the same amount of total strain as that in the ferrite phase. Because the elastic deformation of the cementite phase is limited, the plastic deformability of the cementite in pearlitic steels [5] is directly linked to the ductility mechanism of the pearlitic steel.

In general, a bare specimen of millimeter-sized cementite exhibits brittle properties [6], whereas plastic deformation of cementite in a pearlite microstructure under tensile loading was clearly shown by Tanaka *et al.* using a novel technique involving precision markers [7]. Ohashi *et al.* investigated a possible mechanism of stable plastic deformation of cementite in the microstructure by using finite element analyses [8]. They suggested that when ferrite sandwiched by submicrometer-sized cementite exhibited higher values of yield stress and strain hardening, the concentration of plastic deformation in cementite was effectively suppressed and stable plastic deformation was realized. However, for the cementite to deform plastically, a sufficient number of dislocations necessary for plastic deformation should be generated or supplied. In the case of plastic deformation of nanostructured materials divided by interfaces at nanometer intervals, most dislocations are generated from the interfaces [9-11]. Similarly, dislocations in the cementite layer are considered to be supplied from the heterointerfaces between ferrite and cementite layers. Plastic deformation first occurs in ferrite layers [3,12,13], and the supply of dislocations into cementite layers by dislocation transmission through the heterointerfaces should be possible. In this study, we employ an atomistic approach to evaluate this possibility.

The crystal structure of cementite has been shown to be orthorhombic [14], and some atomic potentials have been proposed [15-17]. However, the atomic structure of the dislocation core has not yet been elucidated, and the detailed atomic structure at the

heterointerface between cementite and ferrite layers remains an unresolved topic. Therefore, in this study, we use generalized and simplified crystal structures and mechanical properties rather than attempting to establish these parameters for actual materials. We focus on obtaining general understandings of the role of the heterointerface in the plastic deformation of multilayered composites of brittle and ductile materials.

Whether a material is ductile or brittle can be determined from fundamental mechanical properties of the material [18], which enables us to design a virtual material by controlling the shape of an atomic potential. In this study, we use artificially designed atomic potentials to develop model materials with ductile or brittle properties. The interatomic bonding strength between atoms positioned near the heterointerface is also considered to play a key role in the deformation of brittle layers. Atomic interactions near the interface are systematically changed over a wide range, and we examine the effect of the interface strength.

The structure of this paper is as follows. First, in section 2.1, we describe our design of two virtual materials with either ductile or brittle properties on the basis of the concepts of ideal strength and stress intensity factor, and employ a two-dimensional triangle-lattice system. Second, in section 2.2, to control the mechanical properties of the heterointerface region, we introduce heterointerface potentials via mixtures of interatomic potentials for brittle and ductile phases. Using this approach, we can control the interatomic bonding strength at the heterointerface. Then, in section 3.1, we investigate the influence of the interface strength on the dislocation transmission phenomena, and in section 3.2, we examine the role of the heterointerface on the mechanical properties of multilayered composite models. Finally, in section 4, we discuss the coexistence of high strength and ductility of drawn pearlitic steels in terms of the roles of the heterointerface and heterointerface-mediated plastic deformation in multilayered composite models found in our atomic simulations.

2. Numerical models for multilayered composite materials

2.1 Material design for ductile and brittle phases

A two-dimensional triangle-lattice system and the Morse potential [19], which is a two-body interatomic potential, are adopted to express virtual materials with a generalized and simplified crystal structure and mechanical properties. The function is expressed as follows:

$$\Phi(r) = D\{\exp[-2\alpha(r - r_0)] - 2\exp[-\alpha(r - r_0)]\}. \quad (1)$$

where r represents the interatomic distance between two atoms. To reduce the computational cost, we introduce a cut-off distance “ r_c ” of 0.6 nm by modifying the function of $\Phi(r)$ into the shifted-force potential $\phi(r)$ as follows [20]:

$$\phi(r) = \begin{cases} \Phi(r) - \Phi(r_c) - [r - r_c] \left(\frac{d\Phi}{dr} \right)_{r_c}, & r \leq r_c \\ 0, & r > r_c. \end{cases} \quad (2)$$

where D , α , and r_0 are tunable parameters closely related to the cohesive energy, the elastic moduli, and the lattice constant, respectively. In this study, we attempt to design virtual materials with either ductile or brittle properties by controlling these parameters on the basis of dimensionless values of $\mu b/\gamma_s$, where μ , b , and γ_s are the shear modulus, the Burgers vector, and the surface energy, respectively.

The dimensionless value of $\mu b/\gamma_s$ has been reported to approximately determine the inherent mechanical properties of single-phase materials, i.e., ductile or brittle properties [18]. Two physical descriptions determine the threshold value of $\mu b/\gamma_s$. One is the relationship between the ideal tensile strength [21] and ideal shear strength [22], and the other is the relationship between two stress intensity factors for brittle cleavage [23] and dislocation nucleation [24] from the crack tip. In general, if $\mu b/\gamma_s$ is greater than approximately 10, the material tends to exhibit brittle properties; in contrast, if $\mu b/\gamma_s$ is less than approximately 10, the material tends to exhibit ductile deformation [18].

On the basis of the concept of $\mu b/\gamma_s$, we designed 22 different virtual materials with $\mu b/\gamma_s$ values that ranged from 4 to 26. To confirm the validity of $\mu b/\gamma_s$ for the material design in atomic simulations, we investigate the relationship between deformation modes and $\mu b/\gamma_s$ by performing tensile loading tests for the virtual materials with a perfect structure; the results of which are shown in Fig. 1. The analysis temperature is kept constant at 10 K. The strain rate is 4×10^8 1/s, and periodic boundary conditions are adopted in all directions. For each virtual material, five cases of tensile simulations are performed with different initial velocity distributions. The squares, circles, and triangles in Fig. 1 represent the brittle-fracture mode in all cases, the ductile deformation mode in all cases, and the brittle or ductile mode in each case, respectively. Detailed deformation mechanisms for each mode are described in the following paragraphs. These results suggest that the virtual material designed here exhibits ductility and brittleness when $\mu b/\gamma_s$ is less than 12 and greater than 16, respectively. This tendency corresponds well to the proposed threshold value of $\mu b/\gamma_s \approx 10$.

The use of brittle and ductile virtual materials with the same lattice constant to simplify the mechanical phenomena around the heterointerface between brittle and ductile phases is reasonable because the influence of the lattice mismatch does not need to be considered. Therefore, in this study, we employ two virtual materials with $\mu b/\gamma_s = 5.7$ as the ductile phase (M-D) and $\mu b/\gamma_s = 17.3$ as the brittle phase (M-B) because they show the maximum $\mu b/\gamma_s$ difference among any pairs of virtual materials shown in Fig. 1 under the condition of identical lattice constants.

We here describe the material properties and defect evolutions of M-D and M-B under tensile loading. Table 1 shows the material properties of M-D and M-B. In the two-dimensional triangle-lattice system, C_{11} represents the elastic constant of the perpendicular direction against the close-packed plane. The Cauchy relation ($C_{12} = C_{44}$) necessarily holds because of the adopted central two-body interatomic potential. Parameter γ_s represents the surface energy for the close-packed plane. All of the elastic constants of M-B are greater than those of M-D; however, the surface energy of M-B is lesser than that of M-D. Hence, it follows that M-D has a more ductile nature than M-B. Figure 2 shows the defect evolution of two single-phase models of M-D and M-B under

tensile loading simulations. Figure 2(a) shows the first plastic phenomenon of M-D under tensile loading when $\varepsilon = 0.1772$; that is, when homogeneous dislocation nucleation occurs [26]. In case of M-B, the same nucleation is observed when $\varepsilon = 0.1512$. After the first dislocation nucleation, M-D can plastically deform by the movement of dislocations and exhibits ductility; therefore, the M-D model does not show brittle fracture under the tensile loading conditions. In contrast, M-B shows cleavage fracture from the microcrack nucleated by the dislocation interactions, as shown in Figs. 2(b)–(d). One reason for the different behaviors of M-D and M-B may be the surface energy. Because the surface energy of M-B is much smaller than that of M-D, as shown in Table 1, geometrical misfits generated by dislocation interactions in M-B are accommodated by the nucleation of new surfaces, which act as the starting point of cleavage fracture.

2.2 Material design for mechanical properties of heterointerfaces

We construct a multilayered composite material by combining the two designed materials: M-D and M-B; therefore, heterointerface regions appear at the boundary between two phases. To express the interatomic bonding strength between atoms near the heterointerface, we introduce heterointerface potentials $\phi_{BD}(r)$ expressed by mixtures of interatomic potentials $\phi_D(r)$ for M-D and $\phi_B(r)$ for M-B. In this study, the simplest mixture rule shown in Eq. (3) is adopted, which allows us to systematically change the interatomic bonding strength by controlling an adjustable parameter A .

$$\phi_{BD}(r) = \frac{\phi_B(r) + \phi_D(r)}{A}. \quad (3)$$

If A takes a value of 2, the mixture rule is the same as the arithmetical mean. The shapes of $\phi_D(r)$, $\phi_B(r)$, and $\phi_{BD}(r)$ are shown in Fig. 3. In this study, we set A to values in the 1–5 range to express a wide range of the interface strength, which increases with decreasing A . The curvatures of $\phi_{BD}(r)$ govern the elastic properties of heterointerface regions; hence, the elastic constants around the interface region also increase with decreasing A . The determination of the exact elastic constants of interface regions is not easy; however, a simple estimation can be calculated using the equation $(C_{ij,D} + C_{ij,B})/A$, which is the same analogy of the simple mixture rule of Eq. (3). In addition, heterointerface energy is also controlled by A . Because plastic deformation phenomena

around the heterointerface are influenced by mechanical properties of the heterointerface region, we investigate the role of the heterointerface on the ductility of multilayered composites by changing the value of A .

2.3 Analysis models and conditions

Before investigating the role of the heterointerface on the ductility of multilayered composites, which is described in section 3.1, we first investigate the influence of heterointerface strength on the fundamental plastic phenomenon of dislocation transmission across the heterointerface from ductile to brittle phase using model I, which is shown in Fig. 4(a). The misorientation angle θ^I of the heterointerface in model I is 21.8° , and the structure shows a symmetric tilt grain boundary. The force field of the heterointerface region within $2r_c$ is expressed by the term $\phi_{BD}(r)$ in Eq. (3). Dislocations are impinged into the heterointerface from the ductile phase in advance by artificially generating a dislocation dipole in the ductile phase under pretensile loading. We apply tensile deformation tests to model I with various values of A at a strain rate of 2×10^8 1/s and a temperature of 10 K. The dimensions L_y^I , L_B^I , and L_D^I of model I are 47.5 nm, 24 nm, and 24 nm, respectively.

In section 3.2, we investigate the role of the heterointerface on the mechanical properties of multilayered composite materials using model II, which is shown in Fig. 4(b). The close-packed plane, i.e., a cleavage plane, of the M-B phase is set to be perpendicular to the tensile loading axis. The crystal orientation of the M-D phase is set to take a misorientation angle θ^{II} of 30° ; therefore, the heterointerface structure shows an asymmetric tilt boundary. In model II, we introduce one and eight initial defects into the M-B and M-D phases by removing three atoms for each defect, respectively, as shown in Figs. 5(a) and 5(b). After the relaxation process at 10 K, the initial defect structure in the M-B phase with low surface energy is maintained as a crack, which is expected to act as a starting point of brittle fracture, and the initial defect structures in the M-D phase with high surface energy change into dislocation dipoles, as shown in Fig. 5(c). Hence, we can expect that the first plastic deformation occurs from the ductile phase. We perform tensile deformation tests in the y -direction to model II with different values of A at a strain rate of 4×10^8 1/s and a temperature of 10 K. The

dimensions L_y^{II} , L_B^{II} , and L_D^{II} of model II are 100 nm, 50 nm, and 50 nm, respectively.

For both models, periodic boundary conditions are adopted in all directions. During the tensile deformation in the y -direction, the dimensions in the x -direction of both models are controlled to keep the normal stress σ_x at zero [27], and the analysis temperature is maintained at 10 K by the velocity scaling method [28].

3. Results

3.1 Dislocation transmission phenomena through heterointerfaces with different bonding strengths

Figure 6 shows the relationship between the heterointerface strength governed by A in Eq. (3) and the critical stress for dislocation transmission through the heterointerface. The transverse axis represents the normalized heterointerface energy: $E_{\text{int}} / (\gamma'_{\text{s,D}} + \gamma'_{\text{s,B}})$, which increases with A . Here E_{int} is the heterointerface energy with no lattice dislocation, and $\gamma'_{\text{s,D}}$ and $\gamma'_{\text{s,B}}$ are the surface energy values for the same crystal orientation of the heterointerface in model I. The values of $\gamma'_{\text{s,D}}$ and $\gamma'_{\text{s,B}}$ are 2.78 J/m² and 1.58 J/m², respectively. If the normalized heterointerface energy takes a value of 1, the heterointerface acts as a surface. In contrast, if the normalized heterointerface energy takes a negative value, the heterointerface becomes more energetically stable than each single phase. The increase in the critical stress with the normalized heterointerface energy is clearly observed in Fig. 6; therefore, dislocation transmission through the heterointerface becomes easier as the interatomic bonding strength increases at the heterointerface. We find two characteristic phenomena that control the dislocation transmission in this system: one is dislocation-core decomposition in the heterointerface region; the other is the heterointerface decomposition into the phase boundary (between the ductile and brittle phases with no misorientation angle) and the grain boundary (with θ^{I} in the ductile phase). Explanatory details are provided in the following paragraphs.

The first phenomenon is dislocation-core decomposition. Figures 7(a) and 7(b) show the shear stress distributions just before the dislocation emission from the

heterointerface with $A = 1.25$ and $A = 3$, respectively. The black atoms represent the defect structure. The shear stress field around the dislocation in the case of $A = 3$ spreads much more than that in the case of $A = 1.25$. This increased spread of the shear stress might be due to the dislocation-core decomposition at the heterointerface with weak interatomic bonding. When one of the decomposed dislocations transmits through the heterointerface, a residual Burgers vector at the transmission place becomes larger than the case of no decomposed dislocation; therefore, the dislocation transmission through the heterointerface becomes difficult when interatomic bonding strength is weak. The same tendency has also been observed in an atomic simulation of the relationship between the resistance to slip transmission across Cu/Nb interfaces and the interface shear strength [29].

The second phenomenon is heterointerface decomposition. Figures 7(c) and 7(d) show the atomic structures just after the dislocation emission from the heterointerface with $A = 1.25$ and $A = 3$, respectively. Here the black atoms represent the defect structure; hence, the defect atoms construct the grain boundary with θ^I . The pink and light-blue atoms represent the perfect structure in the ductile and brittle phases, respectively; hence, we can identify the position of the phase boundary with/without the misorientation angle. In the case of $A = 3$, as shown in Fig. 7(d), the grain boundary and the phase boundary take the same position. However, in case of $A = 1.25$, as shown in Fig. 7(c), the positions of the two boundaries differ; therefore, grain boundary migration occurs. This positional difference can be observed in a range of A from 1 to 2, and the positional gap between two boundaries is approximately 0.35 nm. Because the interatomic bonding strength of the heterointerface region increases with decreasing A , it is energetically disadvantageous to construct defect structures at the heterointerface with small values of A . Moreover, the grain-boundary energies with the same crystal orientation of M-D and M-B are 0.85 J/m² and 1.06 J/m², respectively; hence, the construction of a grain boundary with θ^I is easier in the ductile phase than in the brittle phase. This result indicates that the dislocation is emitted from the grain boundary with θ^I in the ductile phase instead of from the heterointerface with θ^I . Under the constant strain condition, the phase boundary region with the coherent structure has a larger tensile stress value than the grain boundary region because the elastic constants of the phase boundary region are larger than those of each single phase region when A is

small; hence, the large resolved shear stress field in the phase boundary region could assist the dislocation emission from the grain boundary. Consequently, heterointerface decomposition facilitates the dislocation transmission.

3.2 The role of the heterointerface on the mechanical properties of multilayered composite materials

In the previous section, we confirmed that heterointerface strength can control the dislocation transmission phenomenon through the interface; i.e., plastic deformation potential of heterointerface improves with heterointerface strength. In this section, we investigate the role of the heterointerface on the mechanical properties of multilayered composite materials using model II with $A = 1, 1.4, 2$, and 5 . Figure 8 shows the stress–strain curves of model II with different values of A , and the curves of single-crystal models of M-D and M-B with the same crystal orientation as that in model II. The initial defects in each single-crystal model are also the same as those in model II. Each curve is shown until the fracture strain, at which point the brittle phase forms a complete tunnel-crack terminated by heterointerfaces. The fracture strain clearly increases with decreasing A despite a small decrease in the peak stress. Consequently, this simulation suggests that it is possible to obtain a coexistence of strength and ductility in multilayered composite materials under the constant strain condition when the heterointerface region has high plastic deformation potential.

Figure 9 shows the evolution of defect structures in multilayered composite models with various interface strengths. The black atoms represent defect structures, and other colors represent the values of atomic shear stress of τ_{xy} . Figure 9(a) shows the shear stress distribution of model II with $A = 5$ when ε is 0.02 . Large $|\tau_{xy}|$ fields in the M-D phase are due to edge dislocations, as shown in Fig. 9(b). In all models, plastic deformation occurs first from dislocation dipoles in the ductile phase when ε reaches 0.02 and when all slopes of the stress–strain curves deviate from the Young’s modulus of model II, as shown in Fig. 8. Most dislocations are impinged into heterointerfaces when ε is 0.03 , as shown in Fig. 9(b). After dislocation impingements into the heterointerface, the stress–strain curve linearly increases again with a slope that differs from that of the Young’s modulus of model II because of the different plastic strain

between the M-D and M-B phases. This change in slope of the stress–strain curve for multilayered composites has also been confirmed in the continuum model [8]. To this point, all the models developed in this study have shown the same defect evolution. However, after further tensile deformation, the defect evolution differs between models because of different roles of heterointerfaces.

First, we consider the case of a heterointerface with a low plastic deformation potential: $A = 5$. Because no dislocation emission occurs from the heterointerface to the brittle phase until peak stress, the tensile stress in the M-B phase linearly increases and finally reaches a critical value for the cleavage from the central crack tip in the M-B phase, as shown in Fig. 9(d). Therefore, the multilayered composite material with a heterointerface that exhibits weak plastic deformation potential shows high peak stress but small elongation. In this case, the dominant role of the heterointerface in determining the mechanical properties of the multilayered composite is the strong barrier to dislocation motion in the ductile phase.

Next, we consider the case of a heterointerface with a high plastic deformation potential: $A = 1$. As shown in Fig. 9(c), when $\varepsilon = 0.04$, dislocations are emitted from the heterointerface toward the brittle phase, and the stored elastic energy in the M-B phase can subsequently be released. Consequently, reaching critical stress for cleavage fracture in the brittle phase is not easy; hence, the multilayered model with the heterointerface with high plastic deformation potential shows much better ductility than the other models, as shown in Fig. 9(f). In this case, the dominant role of the heterointerface on the mechanical properties of the multilayered composite is the dislocation source of the brittle phase.

Finally, we consider the case of the heterointerface with intermediate plastic deformation potential: $A = 1.4$. In this case, dislocation emissions from the heterointerface occur before the cleavage fracture starts from the central crack tip in the brittle phase. However, other cleavage fractures occur at the heterointerfaces, as shown in Fig. 9(e). The fracture mechanism is as follows. In the equilibrium state of model II, heterointerface decomposition occurs into the asymmetrical grain boundary with θ^{II} and into the phase boundary. Under tensile loading, a portion of the grain boundary

migrates toward the phase boundary to transform its structure into a stable symmetrical grain boundary; hence, the boundary plane takes a wavy shape with symmetrical and asymmetrical components, as shown in Fig. 9(e). Because the locations from which dislocations will be emitted become very close to the phase boundary, the geometrical misfit of the residual Burgers vector forms in the vicinity of the brittle phase after the dislocation emission. As shown in Fig. 6, a larger tensile loading value is required to emit a dislocation from the heterointerface with intermediate plastic deformation potential ($A = 1.4$) than from the interface with high plastic deformation potential ($A = 1$). The larger tensile loading in model II ($A = 1.4$) leads to the cleavage fracture from the geometrical misfit at the phase boundary; hence, the multilayered composite shows greater strength but smaller elongation than that with high plastic deformation potential ($A = 1$). In this case, the dominant role of the heterointerface on the mechanical properties of the multilayered composite is to supply the starting points for the cleavage fracture.

Consequently, our simulations suggest two necessary conditions for the heterointerface to achieve both strength and ductility in multilayered composite materials under the constant strain condition. The first condition is sufficient plastic deformation potential to supply dislocations in brittle phases for their plastic deformation in order to not generate brittle fracture in brittle phases. The second condition is sufficient accommodation potential for the geometrical misfit of the residual Burgers vector created by the dislocation emission from the boundary in order to not generate brittle fracture at the heterointerface.

4. Discussion

The main findings of our simplified atomic simulations are as follows: the more the interface strengthens, the more dislocation transmission through the interface eases i.e., the heterointerface with strong interatomic bonding strength can supply a sufficient number of dislocations into the brittle phase. This phenomenon finally improves the ductile properties of our designed multilayered composites of brittle and ductile materials. Herein, we discuss the ductile mechanisms of line-drawn pearlitic steels based on the results obtained in this atomistic study and our continuum analyses [8].

The line-drawing process of pearlitic steels is well known to effectively enhance the strength of the resulting steels, although their elongation in tensile tests is diminished [30]. This relationship is understood as a trade-off between strength and ductility. The origin of such mechanical behavior in line-drawn pearlitic steels can be deduced to some microstructural changes such as a decrease in the lamellar spacing, an increase in the dislocation density, and a supersaturated carbon concentration in ferrite lamellae due to cementite decomposition [31,32]. Recently, a microstructural characteristic induced by a heavily line-drawn process has been reported: the carbon concentration gradually changes from the ferrite phase to the cementite phase, and the carbon concentration in the cementite phase decreases from 25 at.% of the stoichiometric concentration to 17 at.% [33]. On the basis of the experimental facts, the near-field regions of the heterointerface may have difficulty maintaining their original structure and strength when subjected to a line-drawn process.

However, an annealing process has been reported to drastically improve the ductility of line-drawn pearlitic steels despite the fact that the decrease in their yield strengths is small [3]. This process should cause little change in the lamellar spacing, but we can expect a decrease in dislocation density as well as the recovery of carbon concentration from an abnormally supersaturated state to a normal equilibrium state. The carbon concentration recovery suggests that the heterointerface structure and strength are also recovered to the thermal equilibrium states observed in patented pearlitic steel. Consequently, dislocation density in the ferrite phase and the structure and strength of the heterointerface are expected to be important factors in elucidating the ductile mechanisms of line-drawn pearlitic steels.

First, with respect to the influence of dislocation density on the ductility of pearlitic steel, the continuum simulations using finite element analyses suggest that the high strain hardening potential of the ferrite phase could effectively suppress the concentration of plastic deformation in cementite [8]. The strain hardenability in the ferrite phase should be recovered by the decreased dislocation density induced by the annealing process. Consequently, stable plastic deformation of cementite in terms of the mechanical properties of the ferrite phase is realized through an annealing process.

The next problem to be discussed is the influence of the heterointerface structure and strength on the ductility. We address this issue in terms of the role of the heterointerface discovered during the course of our atomic simulations of multilayered composite models. The multilayered model with low plastic deformation potential at the heterointerface due to weak interatomic bonding strength shows a large yield stress and small elongation. This tendency corresponds well with as-drawn pearlitic steel. However, the multilayered model with high plastic deformation potential at the heterointerface due to strong interatomic bonding strength exhibits greater elongation with slightly lower yield stress. This tendency may correspond well with that of annealed pearlitic steel. These results suggest that the heterointerfaces in as-drawn pearlitic steel have a lower plastic deformation potential than those in annealed pearlitic steel i.e., a heavily line-drawn process probably increases the resistance of the dislocation transmission through the heterointerface from the ferrite to the cementite phase.

A possible mechanism for the large resistance to dislocation transmission by a heavily line-drawn process is as follows: if the heterointerface structure largely deviates from the original structure and approaches an amorphous structure when subjected to a heavily line-drawn process, the interfacial strength, which is closely related to elastic constants, probably decreases. Hence impinged dislocation-core structures could easily spread out at the heterointerface. The resistance to dislocation transmission through the heterointerface may subsequently increase, and the heterointerface cannot function as the dislocation source of the cementite phase. This tendency of dislocation-core decomposition at the heterointerface is the same as that of the weak interatomic bonding strength observed in Fig. 7(b). Consequently, our simple atomic simulation leads to the hypothesis that a heavily line-drawn process changes the role of the heterointerface in determining the ductility of pearlitic steel i.e., cementite decomposition decreases the plastic deformation potential of the heterointerface, which results in as-drawn pearlitic steel exhibiting high strength but low ductility.

In this study, because we adopt a simple two-dimensional triangle-lattice system to simplify heterointerface-mediated plastic deformation, we do not consider the

influence of solute atoms, which result from cementite decomposition, on the ductility of pearlitic steel. However, the dislocation mobility in the ferrite phase can be reasonably considered to be diminished by the high carbon concentration in the vicinity of the heterointerface in ferrite; as such, dislocation transmission through the heterointerface also becomes difficult. This phenomenon does not contradict our suggestion that cementite decomposition decreases the plastic deformation potential of the heterointerface.

5. Summary

In this study, to investigate the role of the heterointerfaces in determining the ductility of heavily-drawn-pearlitic steel, we performed tensile deformation tests of multilayered composite materials brittle and ductile phases with different strengths of the heterointerface between. The results obtained are as follows:

1. Two types of virtual materials with either ductile or brittle properties were designed in the form of a two-dimensional triangle-lattice system based on the dimensionless value of $\mu b/\gamma_s$. The introduced heterointerface potential could control interatomic bonding strength in heterointerface regions.
2. The resistance to dislocation transmission through the heterointerface decreased as interatomic bonding strength at the heterointerface increased. This tendency was explained by considering two phenomena that occur at the heterointerface: dislocation-core decomposition and heterointerface decomposition.
3. The dominant role of the heterointerface in determining the mechanical properties of multilayered composite models was changed by the interface strength. In the case of strong interface strength, the heterointerface acted as dislocation sources of the brittle phase by dislocation transmission through the heterointerface; hence, the multilayered composite model showed good ductility with a small decrease in strength. However, in the case of weak interface strength, the heterointerface acted as a strong barrier to dislocation motion in the ductile phase or as a starting point of the cleavage fracture; hence, the multilayered composite model showed high strength but extremely low

ductility.

4. By comparing the results of atomic simulations with experiments, we hypothesized that cementite decomposition by a heavily line-drawing process decreases the plastic deformation potential of the heterointerface.

5. Our simple atomic simulations suggested two necessary conditions for the heterointerface to simultaneously achieve both high strength and ductility. One condition is sufficient plastic deformation potential to supply dislocations in brittle phases for their plastic deformation. The other is a sufficient accommodation potential for the geometrical misfit generated after dislocation emissions into the brittle phase from which cleavage fracture occurs at the heterointerface.

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Table 1. Mechanical properties for the designed virtual materials M-D and M-B. The

dimensionless value of $\mu b/\gamma_s$ implies the inherent mechanical properties of single-phase materials. The Young's modulus E and the shear modulus μ are estimated by the Voigt approximation [25].

Fig. 1. Relationship between deformation modes and $\mu b/\gamma_s$ under tensile loading of two-dimensional virtual materials.

Fig. 2. Defect configurations of designed ductile (M-D) and brittle (M-B) materials under tensile loading. (a) Homogeneous dislocation nucleation in M-D when $\varepsilon = 0.1772$; (b), (c), and (d) Nucleation of a crack by dislocation interactions in M-B ($\varepsilon = 0.1588$, $\varepsilon = 0.1592$, and $\varepsilon = 0.2316$, respectively.)

Fig. 3. Shapes of interatomic potentials to express the virtual ductile (M-D) and brittle (M-B) materials. For M-D, $D = 16.31999 \times 10^{-20}$ J, $\alpha = 9.75282$ 1/nm, and $r_0 = 0.271327$ nm. For M-B, $D = 8.10001 \times 10^{-20}$ J, $\alpha = 18.40739$ 1/nm, and $r_0 = 0.253051$ nm. The green lines represent the heterointerface potentials. The interatomic bonding strength in heterointerface regions is governed by parameter A in Eq. (3).

Fig. 4. Analysis models I and II used to investigate (a) dislocation transmission phenomena through heterointerfaces with different interatomic bonding strengths and (b) the role of the heterointerface on the ductility of multilayered composite material. Models I and II have symmetric and asymmetric heterointerfaces, respectively.

Fig. 5. Initial atomic configurations of introduced cracks in (a) the brittle phase and (b) the ductile phase. After relaxation calculations, the crack in the brittle phase does not change defect morphology; however, the initial crack in the ductile phase changes the structure into the dislocation dipole shown in (c).

Fig. 6. Relationship between the critical stress to dislocation transmission across the heterointerface from the ductile to brittle phases and the normalized heterointerface energy by surface energies. Values of A are related to heterointerface energy because A controls the interatomic bonding strength at the heterointerface region, as shown in Eq. (3).

Fig. 7. Shear stress distributions around the dislocation at the heterointerface with (a) $A = 1.25$ and (b) $A = 3$ immediately before emission into the brittle phase. Dislocation-core decomposition occurs at the weak boundary shown in (b). Atomic configurations immediately after the dislocation emission from the heterointerfaces with (c) $A = 1.25$ and (d) $A = 3$. Pink and light-blue atoms represent the perfect structure in the ductile and brittle phases, respectively, and black atoms represent defect structures. Heterointerface decomposition occurs at the strong boundary shown in (c).

Fig. 8. Stress–strain curves for multilayered composites with different interface strengths based on the single brittle phase model (M-B) and the single ductile phase model (M-D). Each curve is shown until the fracture strain, at which point the brittle phase forms a complete tunnel-crack terminated by heterointerfaces.

Fig. 9. Development of defect structures of multilayered-composite models under tensile deformation. Black atoms represent defect structures, and other colored atoms represent the values of the shear stress component in the perfect structure. (a) $A = 5$ when $\varepsilon = 0.02$, (b) $A = 5$ when $\varepsilon = 0.03$, (c) $A = 1$ when $\varepsilon = 0.04$, (d) $A = 5$ when $\varepsilon = 0.08$, (e) $A = 1.4$ when $\varepsilon = 0.1$, and (f) $A = 1$ when $\varepsilon = 0.08$. (g) Burgers circuit for an edge dislocation in the ductile phases in (a).

Table 1

	lattice constant a_0 (nm)	cohesive energy E_c (eV)	elastic constant C_{11} (GPa)	elastic constant $C_{12}=C_{44}$ (GPa)	Young's modulus E (GPa) (Voigt average)	shear modulus μ (GPa) (Voigt average)	surface energy γ_s (mJ/m ²)	$\mu b/\gamma_s$
M-D	0.2493	-2.488	182	60.7	151.7	60.7	2647	5.7
M-B	0.2493	-1.579	307	102.5	256	102.4	1473	17.3

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