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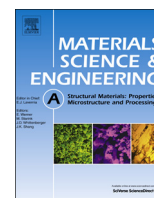
A multiscale approach for the deformation mechanism in pearlite microstructure: Atomistic study of the role of the heterointerface on ductility

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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.

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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 the 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

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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:

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

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]:

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

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 $4 \times 10^8 \text{ s}^{-1}$, 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-
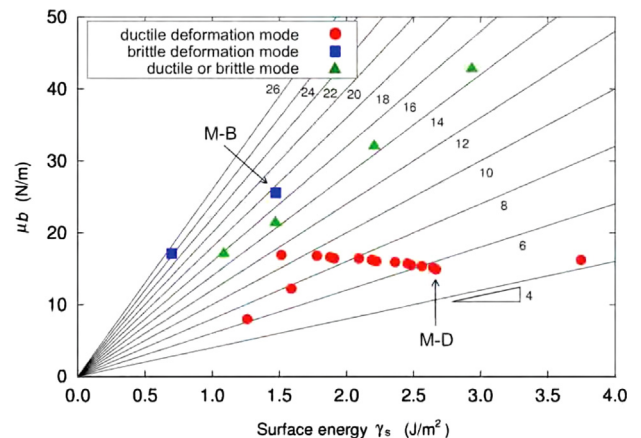

Fig. 1. Relationship between deformation modes and $\mu b/\gamma_s$ under tensile loading of two-dimensional virtual materials.