Influence of Interfacial Mechanical Properties on Elongation of Multilayered Composite Metals

Tomotsugu Shimokawa[1,*]

[1] School of Mechanical Engineering, Kanazawa University, Kakuma-machi, Kanazawa, Ishikawa 920-1192, Japan
* Corresponding author: simokawa@t.kanazawa-u.ac.jp

Abstract Multilayered composite metals (e.g., pearlitic steels) composed of alternating layers of cementite and ferrite show unique and excellent mechanical properties, such as coexistence of strength and ductility. In this study, we investigate the influence of interfacial mechanical properties on the elongation of multilayered composite metals through molecular dynamics simulations. When the interface has weak interatomic bonding, it is difficult for mobile dislocations to transmit through the interface. Thus, the multilayered model shows small elongation due to the cleavage of the brittle phase under large tensile stress by stress partitioning between the brittle and ductile phases. On the other hand, when the interface has strong interatomic bonding, dislocations can easily transmit through the interface and thus the multilayered model displays larger elongation.

Keywords Interface, Dislocation, Crack, Atomic Simulation, Mechanical Property

1. Introduction

Generally, the strength and ductility of pearlitic steel containing lamella structures with random orientations can be improved by a line drawing process. However, when drawing strain becomes greater than 1 and the lamella structures are oriented parallel to the drawing direction, the strength effectively increases but the ductility begins to decrease. For example, cold-drawn, hypereutectoid pearlitic steel wires with lamellar spacing of less than 10 nm that exhibit cementite decomposition have maximum tensile strength of greater than 6 GPa but have very limited elongation properties [1]. On the other hand, cold-drawn pearlitic steel aged at 698 K and still containing oriented lamella structures exhibit significant uniform elongation [2]. In this case, the cementite decomposition was recovered. It is still unclear how elongation can be improved by this type of annealing process.

In this study, we hypothesized that the interfacial structure is changed by cementite decomposition. We investigated the influence of interfacial mechanical properties on the elongation of multilayered composite metals through molecular dynamics simulations.

2. Virtual Materials with Ductile and Brittle Properties

2.1. Material Design

To model virtual materials with either ductile or brittle properties, we used a two-dimensional triangular lattice system. The interatomic potential of the system is expressed in terms of the Morse potential as follows:

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

Here, r is the distance between two atoms; D, α, and r_0 are controllable parameters and are closely related to the cohesive energy, elastic moduli, and lattice constant, respectively. Moreover, to introduce the cut-off distance, r_c, $\phi(r)$ is modified into the shifted-force potential $\phi_s(r)$ as follows:

$$\phi_s(r)=\begin{cases}\phi(r)-\phi(r_c)-[r-r_c]\left(\dfrac{d\phi}{dr}\right)_{r_c}, & r \le r_c \\ 0, & r > r_c\end{cases} \quad (2)$$

Here, we set r_c to 0.6 nm.

It has been shown that the dimensionless value of $\mu b/\gamma_s$ can roughly determine the inherent mechanical properties of single-phase materials, i.e., ductile or brittle properties [3]. Here, μ, b, and γ_s are the shear modulus, Burgers vector, and surface energy, respectively. If $\mu b/\gamma_s$ is greater than 10, the material generally exhibits brittle properties. On the other hand, if $\mu b/\gamma_s$ is smaller than 10, the material shows ductile deformation. There are two physical descriptions for the threshold value of $\mu b/\gamma_s$. One is the relationship between the ideal tensile strength and ideal shear strength, and the other is the relationship between the stress intensity factors for brittle cleavage and dislocation nucleation from the crack tip.

Table 1 shows the material parameters for two designed virtual materials. The dimensionless values of $\mu b/\gamma_s$ are 6.5 for the virtual material "M-D" and 17.7 for "M-B." Therefore, we can consider the M-D material as a ductile phase and the M-B material as a brittle phase. To simplify the mechanical phenomena around the interface between the brittle and ductile phases, we set the same value for the lattice constant of each model; it is not necessary to consider the lattice mismatch influence.

Table 1. Parameters of designed virtual materials with ductile and brittle properties.

	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 agerage)	surface energy γ_s (mJ/m^2)	$\dfrac{\mu b}{\gamma_s}$	
M-D	0.2493	-2.488	206.6	68.9	172.2	68.9	2645	**6.5**	**ductile**
M-B	0.2493	-1.579	308.7	102.9	257.3	102.9	1452	**17.7**	**brittle**

2.2. Mechanical Properties of Virtual Materials

To confirm the mechanical properties of the single-phase material described by the designed Morse potential, tensile deformation tests were performed at a strain rate of 4×10^8 1/s and 10 K. Figure 1(a) shows stress–strain curves of the two designed virtual materials, M-B and M-D. Defects in the form of micro-cracks are initially introduced into each material by removing three atoms from the perfect structure. The number of micro-cracks is 1 for M-B and 12 for M-D. After relaxation before tensile loading, all initial cracks of M-D changed into dislocation dipoles. This transition should be closely related to the large value of the surface energy of M-D. In the case of M-B, the micro-crack begins to propagate at the peak stress and M-B shows the brittle fracture mode with small elongation. On the other hand, in the case of M-D, yielding occurs by dislocations moving from the dislocation dipoles, and then, M-D displays ductile properties with large elongation. Therefore, it can be confirmed that the $\mu b/\gamma_s$ value can determine the mechanical properties of the simple two-dimensional single-phase materials on the atomic scale. In the following section, we investigate the influence of interfacial mechanical properties on the elongation properties of multilayered composite materials by combining these two virtual materials.

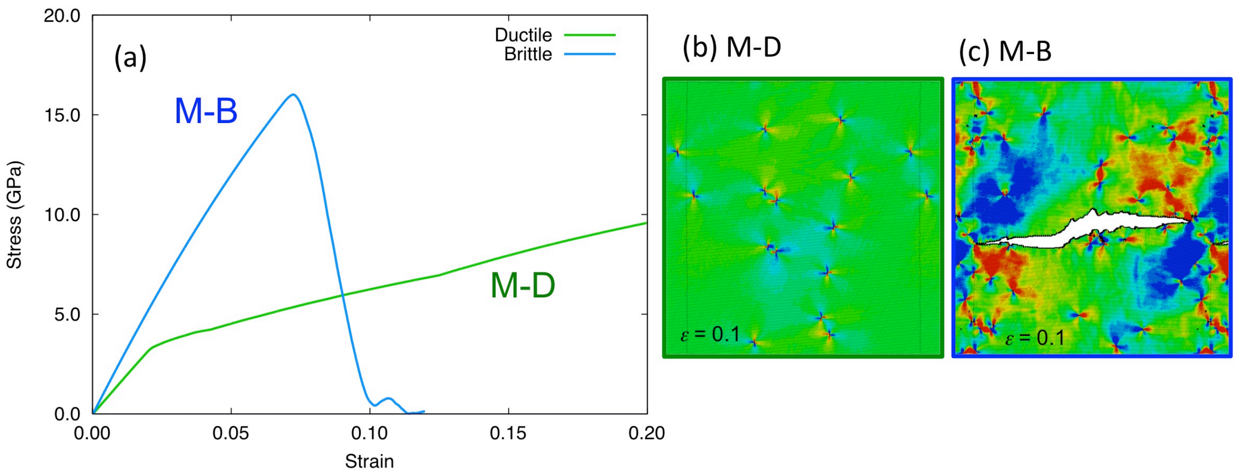

Figure 1. Stress–strain curves of virtual materials with ductile (M-D) and brittle (M-B) properties. (b) and (c) show the shear stress distributions of the single-phase models under tensile loading.

3. Mechanical Properties of Multilayered Composites

3.1. Multilayered Composite Models

Figure 2 shows the analysis model of the multilayered composite consisting of M-B and M-D. The crystal orientation of M-D is rotated 30 degrees from M-B, and thus, the interface has the misalignment angle. Initial micro-cracks are introduced into each phase, and all initial cracks in M-D change their structures into dislocation dipoles after relaxation. Periodic boundary conditions are adopted in all directions and the tensile deformation in the y-direction occurs at a strain rate of 4 × 10^8 1/s and 10 K.

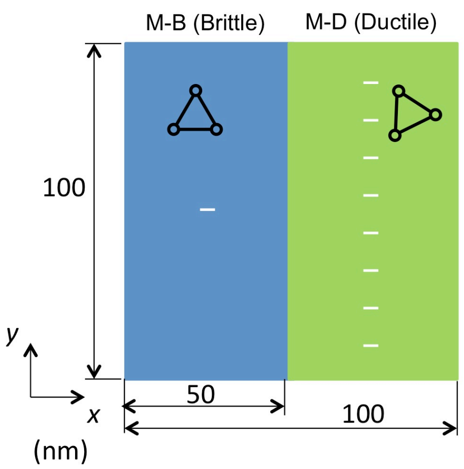

Figure 2. Schematic of the multilayered composite model.

To investigate the influence of interfacial region's mechanical properties on the elongation of multilayered composites, we consider three different types of interatomic bonding strengths between the M-D and M-B phases. The interaction between the M-D and M-B phases $\phi_{BD}(r)$ is calculated by $(\phi_B(r) + \phi_D(r))/A$, where A = 1 (strong bonding strength), A = 2 (normal bonding strength), or A = 5 (weak bonding strength).

3.2. Influence of Interfacial Mechanical Properties on Mechanical Properties of Multilayered Composites

Figure 3 shows the stress–strain curves for single-phase materials and multilayered composite materials with different interfacial bonding strengths. The multilayered composites demonstrate a better combination of strength and elongation than the single-phase materials. It is also apparent that the stronger the interfacial bonding, the larger the peak stress on the multilayered composite model. However, for the elongation, we can see the opposite tendency.

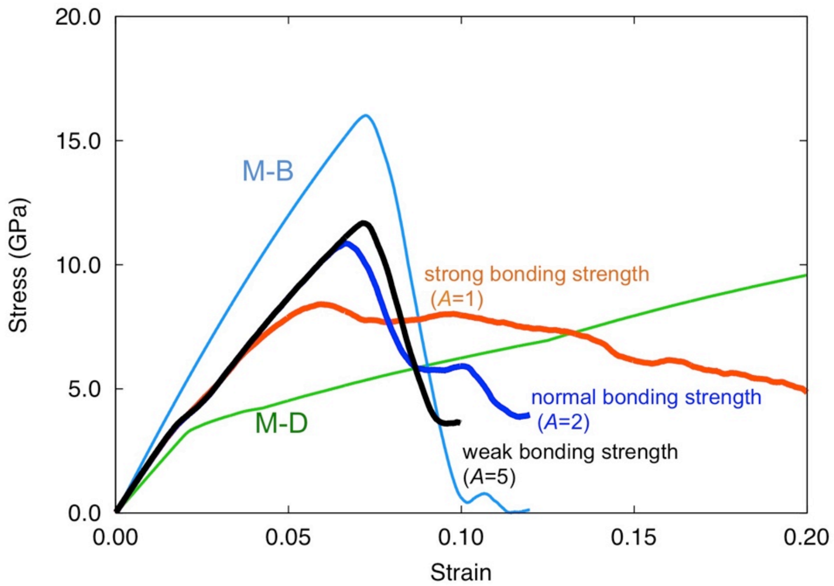

Figure 3. Stress–strain curves of multilayered composites with different interface strengths.

Figure 4 shows the plastic deformation phenomena around the interfacial region with different mechanical properties. Atomic color represents the shear stress component. First, dislocations in the ductile phase move toward the interface in cases of both A = 1 and 5 when ε=0.02. In the case of the weak bonding strength of A = 5, the dislocations are impinged into the interface and further plastic deformation does not occur from the interface. Therefore, initiation of plastic deformation in the brittle phase is delayed. These results show that it is difficult for dislocations from the ductile phase to transmit through the interface when the interfacial region has a weak bonding strength. Consequently, the multilayered model with A = 5 shows high peak stress but small elongation owing to the cleavage of the brittle phase under large tensile stress by stress partitioning between the brittle and ductile phases (see Fig. 4(a)). On the other hand, in the case of a strong bonding strength of A = 1, dislocation emissions can easily propagate from the interface, and thus, plastic deformation propagation occurs from the ductile to brittle phases across the interface. The stored elastic energy in the brittle phases can be released by the plastic deformation. Therefore, it is not easy to reach the critical stress for the cleavage fracture in the brittle phase (see Fig. 4(b)). As a result, the multilayered model with a strong interfacial bonding strength, namely with the interface having the role of the dislocation source, shows much better ductility than the model with a weak interfacial bonding strength. These results imply that it is important to control the interfacial structure to design the multilayered composite metals with coexistence of strength and ductility.

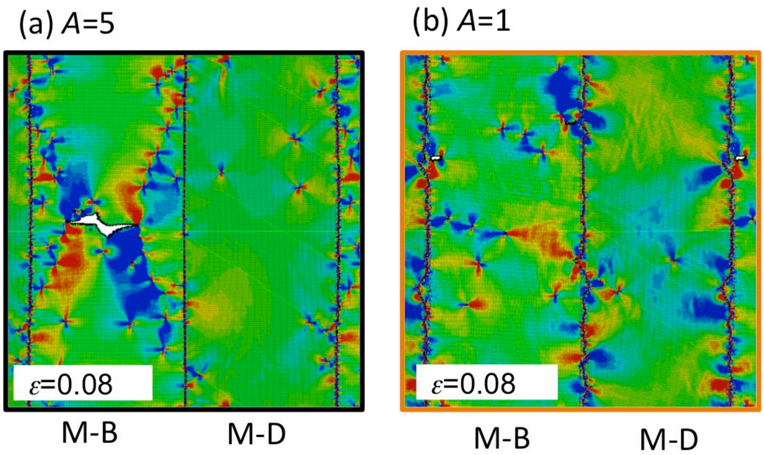

Figure 4. Plastic deformation phenomena around the interface with different mechanical properties.

3.3. Discussion

Heavily drawn pearlitic steel wires having high tensile strength but small elongation exhibit cementite decomposition at the vicinity of the interfacial region. On the other hand, cold-drawn pearlitic steel aged at 698 K exhibits large uniform elongation [2] and the cementite decomposition recovers. This suggests that the interfacial structures between cementite and ferrite phases change by cementite decomposition due to the equilibrium interfacial structure having the maximum solubility of carbon in both phases. In particular, the role of the interface in plastic phenomena in heavily drawn pearlitic steel wires could change from that in aged pearlitic steel.

In our atomic simulations, the multilayered composite model, having a small dislocation source ability of the interface, showed a smaller elongation property than the model having a high dislocation source ability of the interface. This result implies the possibility that the interface structure after cementite decomposition also has a smaller dislocation source ability than that of aged pearlitic steels.

4. Conclusion

We investigated the influence of interfacial mechanical properties on the elongation of multilayered composite metals through molecular dynamics simulations. We designed two-dimensional virtual materials having brittle or ductile properties by controlling the parameters of the Morse interatomic potential. We demonstrated that multilayered composite models with ductile and brittle phases have a superior strength–ductility relationship than single-layered models and that this relationship is closely related to interfacial mechanical properties. These results imply that it is important to control interfacial properties when designing multilayered composite metals with coexistence of strength and ductility.

Acknowledgments

This research was supported by Japan Science and Technology Agency (JST) under Collaborative Research Based on Industrial Demand "Heterogeneous Structure Control: Towards Innovative Development of Metallic Structural Materials."

References

[1] Y. J. Li, P. Choi, S. Goto, C. Borchers, D. Raabe, R. Kirchheim, Acta Materialia, 60 (2012) 4005-4016.
[2] Y. Tomota, P. Lukas, D. Neov, S. Harjo, Y. R. Abe, Acta Materialia, 51 (2003) 805-817.
[3] I. –H. Lin, Journal of Materials Science Letter, 2 (1983) 295.