Nanoindentation Study of Cementite Size and Temperature Effects in Nanocomposite Pearlite: A Molecular Dynamics Simulation

Hadi Ghaffarian^{1,2}, Ali Karimi Taheri¹, Seunghwa Ryu^{*2} and Keonwook Kang^{*3}

¹ Department of Materials Science and Engineering, Sharif University of Technology, Tehran, Iran

² Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology

(KAIST), Daejeon, Korea 305-701

³ Department of Mechanical Engineering, Yonsei University, Seoul, Korea 120-749

*Corresponding Authors: ryush@kaist.ac.kr, kwkang75@yonsei.ac.kr

ABSTRACT

We carry out molecular dynamics simulations of nanoindentation to investigate the effect of cementite size and temperature on the deformation behavior of nanocomposite pearlite composed of alternating ferrite and cementite layers. We find that, instead of the coherent transmission, dislocation propagates by forming a widespread plastic deformation in cementite layer. We also show that increasing temperature enhances the distribution of plastic strain in the ferrite layer, which reduces the stress acting on the cementite layer. Hence, thickening cementite layer or increasing temperature reduces the likelihood of dislocation propagation through the cementite layer. Our finding sheds a light on the mechanism of dislocation blocking by cementite layer in the pearlite.

Keywords: nanoindentation, molecular dynamics simulation, nanocomposite pearlite, cementite size effect, dislocations blocking

1. Introduction

Pearlitic phase, a lamellar structure composed of alternating layers of ferrite and cementite, is a common constituent of steels and plays an important role in determining the mechanical properties of steels, such as toughness, strength and formability [1]. Compared to ferrite, pearlitic structure is known as a harder phase with higher strength due to the presence of cementite lamellae, and its mechanical properties are significantly affected by the cementite microstructure [2-3]. It has been found that the fine pearlite with small interlamellar spacing (~100 nm) and narrow cementite lamellae (~10 nm) shows higher ductility than coarse pearlite during plastic deformation [4-8]. Cementite layer act as a hard obstacle in front of ferrite dislocations and causes to dislocation pile up at the ferrite/cementite interface [9]. However, to the best of our knowledge, there has been no direct experimental or simulation study on the mechanism of the dislocation blockage by the cementite layer.

Nanoindentation is a mechanical test which uses an indenter with a known geometry to plunge into a specific site of the specimen by applying an increasing load [10]. It is widely used to determine the mechanical properties of thin films to clarify the effect of geometric confinement on mechanical properties [11]. In case of carbon steels, nanoindentation techniques have been applied to residual stress calculations in order to determine micro yield stress profile in surface layers [12-13]. Ohmura et al. performed a nanoindentation test on martensitic steel to directly measure matrix strength and separate it from grain boundary effect [14]. It can also be used to elucidate the cementite size effect on the deformation behavior of pearlite phase at nano scales, while complex equipment setup as well as the difficulty in preparing a sample with a desired cementite thickness makes the test costly and time-consuming. These difficulties can be circumvented by employing atomistic simulations.

Molecular dynamics (MD) simulations offer a unique opportunity to investigate the material properties with the desired conditions at nano scale. MD simulation has been widely used to virtually

perform nanoindentation in order to investigate the elastic and plastic deformation mechanisms [15-18]. According to Chang et al. [19], the interlayer graphene thickness can affect the mechanical properties of nickel-graphene nanocomposite as well as indentation depth for dislocation nucleation. Goel et al. [20] have used MD simulations of nanoindentation to compare mechanical properties of Fe_3C (cementite) and Fe_4C iron carbides.

In this study, we perform a series of nanoindentation tests of ferrite-cementite nanocomposites using MD simulations to investigate the role of cementite in blocking dislocation propagation in pearlite structure at various temperatures. For this reason, atomistic models of single crystal ferrite (Fe) film and ferrite-cementite nanocomposite thin films with different cementite thickness are constructed, and subjected to nanoindentation tests with different indenter radii at various temperatures. Our results show that increasing cementite thickness or increasing temperature makes dislocation penetration through the cementite layer harder to occur.

2. Simulation methods

Four ferrite-cementite nanocomposite samples with different thickness of cementite ($P=0, 1, 3$, and 5 layers of cementite unit cells in the x - z plane) were prepared as depicted in Figure 1 to investigate the cementite size effect (the thickness of cementite layer along $[010]_c$) and the temperature effect on the deformation behavior of pearlite under indentation. We chose $[111]_f || [100]_c$, $[\bar{1}10]_f || [001]_c$ and $(11\bar{2})_f || (010)_c$ for the interface orientation relationship between ferrite and cementite according to Bagaryatsky [21] (with regard to cementite lattice constants $a=5.05 \text{ \AA}$, $b=6.69 \text{ \AA}$ and $c=4.49 \text{ \AA}$). Sample dimensions of pure Fe are 15 nm by 15 nm in the x - z plane and 8 nm in the y axis. The thickness of Fe layers is kept constant as 4 nm in pearlite samples, while the thickness of cementite layer is varied as 0.67, 2.0 and 3.35 nm in P1, P3 and P5 samples, respectively. The samples of P0

(pure Fe), P1, P3 and P5 were composed of 165,000, 180,000, 211,000 and 242,000 atoms, respectively. Ferrite and cementite have different lattice structures and lattice constants. The lattice misfit strain in Eq. (1) is relatively large for x and z directions (2.4% and 11.4%, respectively). In order to reduce the in-plane misfit strain in Eq. (2) in x - z plane, the samples were constructed with 30 by 37 ferrite unit cells and 29 by 33 cementite unit cells along x and z directions, respectively. Resultantly, the 0.4% and 0.25% in-plane misfit strains were imposed at the ferrite/cementite interface along x and z directions, respectively.

$$\Delta_{lattice} = \frac{d_{cementite} - d_{ferrite}}{d_{ferrite}}, \quad d: \text{lattice constant} \quad (1)$$

$$\Delta_{in-plane} = \frac{L_{cementite} - L_{ferrite}}{L_{ferrite}}, \quad L: \text{cell dimension} \quad (2)$$

Figure 1. Illustration of pearlite nanocomposite samples; (a) pure Fe, (b) P1, (c) P3 and (d) P5 samples.

The position of cementite layers have been pointed by the back arrows.

The interatomic potential of Fe-C developed by Liyanage et al. [22], based on a modified embedded atom method (MEAM), was used to describe interatomic forces. This potential is fitted to structural, elastic and thermal properties of cementite at a wide range of temperature as well as the surface formation energy, polycrystalline elastic moduli and specific heat obtained from first-principles calculations and experiments [22]. Also, we found that generalized stacking fault energy curves obtained from the MEAM potential are consistent with those obtained from ab initio calculations, as presented in Appendix A. We also have used the potential to investigate the origin of brittle-to-ductile transition of nano-crystalline cementite [23]. The MD simulations were carried out using a parallel MD code, LAMMPS [24] with periodic boundary conditions in x and z dimensions at 100, 300 and 700 K. For each temperature, samples were relaxed for 100 ps under zero pressure with Nose-Hoover isobaric-isothermal (NPT) ensemble. All samples were indented with a constant velocity of 10 m/s along y direction by frictionless spherical indenter. We used three different indenter radii ($R=3$ nm, 5 nm and 7 nm) in order to investigate the effect of indenter radius on the dislocation propagation through the cementite layer. The force on each atom was calculated by:

$$f = \begin{cases} -K(r - R)^2, & r < R \\ 0, & r \geq R \end{cases} \quad (3)$$

where $K=10$ (eV/Å³) is the specified force constant and r is the distance from the atom to the center of the indenter. To prevent translation motion during indentation, we fixed the atoms located in the region within 7 Å from the bottom of sample. The atomic arrangements of the samples, including dislocations, were then visualized using centrosymmetry parameter [25]. The atomic shear strain distribution was also calculated using the method by Shimizu et al. [26].

3. Result and Discussion

Figure 2. Load-displacement curves from nanoindentation tests by indenter with 3 nm radius; (a) pure Fe sample at different temperatures, (b) pearlite structure with different cementite thickness at 100 K and (c) P3 sample indented by different indenter radius at 300 K. The atomistic prediction of load-displacement and Hertzian contact theory are in good agreement until the 1st dislocation nucleation. The insets show the load drop due to first dislocation emission. Arrows in (c) indicate the first dislocation nucleation in the bottom ferrite layer.

Figure 2(a) shows the load-displacement curves of nanoindentation for pure Fe sample indented by 3nm radius indenter at different temperatures. We find that the indentation load gradually increases with the indenter movement up to a certain local maximum and suddenly drops due to dislocation emission from the ferrite region below the indenter tip. In Figure 2(a), the elastic responses are almost identical at different temperatures of 100 to 700 K. Our calculations show that the Young's modulus of ferrite along the loading direction does not change significantly (about 3% decrease), when temperature rises from 100 K to 700 K (see Appendix B for details). We found that measured elastic constants [27, 28] of single crystal Fe decrease by 10% from 100 K to 700 K. While the MEAM potential does not capture the exact amount of thermal softening, our calculations and experimental data are qualitatively consistent in that thermal softening is not significant in the temperature range. Accordingly, the load required for the first dislocation emission does not decrease significantly. However, the increase in temperature leads to the reduction of the indentation load in plastic flow region after the first dislocation emission, and advances the emission of subsequent dislocations due to the thermal softening.

Figure 2(b) shows the load-displacement curves of the samples of Pure Fe, P1, P3 and P5 indented by indenter with 3 nm radius at 100 K. The presence of cementite does not significantly affect the load-displacement curves because the elastic moduli of ferrite and cementite are not appreciably

different [6]. We calculate the indentation load for all samples by the Hertzian theory for semi-infinite thin films,

$$F = \left(\frac{4}{3}\right) E R^{1/2} h^{3/2} \quad (4)$$

where E is the Young's modulus, R is indenter radius and h is indentation depth. The calculated Young's moduli of ferrite and cementite along the loading direction are 203 and 159 GPa at 100 K, respectively (see Appendix B for details). We use the Reuss model to estimate an effective modulus of pearlite elasticity:

$$E = \frac{1}{\frac{\rho_f}{E_f} + \frac{\rho_c}{E_c}} \quad (5)$$

where ρ_f and ρ_c are the volume fractions of ferrite and cementite layers in pearlite. From Eq. (5), the value of effective modulus changes from 198 for P1 to 188 GPa for P5, respectively. As depicted in Figure 2(b), our MD simulation results are in good agreement with prediction from the Hertzian theory before the first dislocation emission. Similar load-displacement behaviors for P1, P3 and P5 samples are observed at 300 K and 700 K.

Figure 2(c) illustrates the load-displacement curves of the P3 sample indented by different indenter radii at 300 K. The larger indenter develops higher indentation load, due to much larger contact area. On the other hand, the increasing indenter radius causes to postpone dislocation emission due to the reduction of stress concentration below the indenter **because the maximum shear stress τ_{max}**

under the indenter is inversely proportional to the $R^{1/2}$. The maximum shear stress from elastic contact mechanics [29] is given by $\tau_{max} = 0.31 \left(\frac{6E^2}{\pi^3 R^2}\right)^{\frac{1}{3}} F^{\frac{1}{3}} = \frac{0.62E}{\pi} \left(\frac{h}{R}\right)^{\frac{1}{2}}$. While the expression is derived for the isotropic materials in the elastic regime, it is also true that the maximum shear stress decreases with indenter radius for the cubic materials. Similar result has been reported by Ruestes et al. for tantalum

indentation [30].

Figure 3. Dislocations evolution after 30 Å indentation of indenter with 3 nm radius in pure Fe, P1, P3 and P5 samples at (a) 100 K, (b) 300 K and (c) 700 K. Out of three pearlite samples, only in P1, dislocations are formed in the bottom ferrite layer. Atoms were colored according to the centrosymmetry parameter values between 1 (blue) and 25 (red) with number of neighbors of 14. Thus, atoms on a perfect BCC lattice were not visualized. Cementite layers are illustrated by black arrows.

In order to understand the effect of cementite thickness on deformation behavior during the indentation, we present atomic configurations showing dislocation evolution after 30 Å indentation by indenter with 3 nm radius in pure Fe, P1, P3 and P5 samples at different temperatures in Figure 3, where the centrosymmetry parameter [25] was applied to screen out atoms on a perfect BCC lattice site. With increasing indentation depth, dislocation loops nucleate below the indenter in the top ferrite layer, and propagate toward the cementite layer. We observe dislocation formation in the bottom ferrite layer

only in P1 sample at 100 K, while in P3 and P5 samples dislocations are completely trapped in the top ferrite layer regardless of imposed temperature.

Depending on the structural details of interface and the relative orientation of slip systems in both crystals across the interface, dislocations can either transmit across the interface or be blocked at the interface. In the case of ferrite-cementite composite, dislocations could rarely pass through the incoherent bcc/orthorhombic interface of Bagaryatski's orientation relationship. The likelihood of dislocation transmission is carefully studied by investigating transmission pathway index χ [31]:

$$\chi = \begin{cases} \cos\left(\frac{\pi}{2} \frac{\theta}{\theta_c}\right) \cos\left(\frac{\pi}{2} \frac{\kappa}{\kappa_c}\right), & \text{if } |\theta| \leq \theta_c \text{ and } |\kappa| \leq \kappa_c \\ 0, & \text{otherwise} \end{cases} \quad (6)$$

where θ is the minimum angle between the intersection lines that each slip plane in ferrite and cementite makes with the interface, κ is the minimum angle between Burgers vectors of slip systems in ferrite and cementite, and θ_c and κ_c are limiting angles of θ and κ for transmission. If the χ of a certain pair of slip systems is equal to or close to unity, the dislocation transmission is favorable at the interface between the two slip systems [32]. According to Eq. (6), when either θ or κ exceeds their corresponding thresholds ($\theta_c=45^\circ$ and $\kappa_c=15^\circ$ [31]), transmission is impossible. Considering main slip systems in ferrite ($\{101\}\langle 11\bar{1} \rangle$ and $\{112\}\langle 11\bar{1} \rangle$) and cementite ($\{100\}\langle 001 \rangle$), there are only 5 distinct geometrically efficient pathways with $\chi > 0.9$ among $24 \times 6 = 144$ possible combinations of slip system pairs (see Table 1). We find that the (110) plane is the slip plane of newly formed dislocation loops in the bottom ferrite layer of P1 sample. According to Table 1, the (110) slip plane does not belong to any possible transmission pathway on ferrite/cementite interface, and the scenario of dislocation transmission can be excluded out. Besides, the higher GSF energy in cementite [33-34] makes the dislocation nucleation in cementite harder than that in ferrite.

Table 1. Efficient transmission pathways for the ferrite/cementite interface of Bagaryatsky orientation relationship.

No.	Slip system in ferrite	Slip system in cementite	χ value
1	$[111](1\bar{1}0)$	$[100](001)$	1
2	$[111](\bar{1}01)$		
3	$[111](0\bar{1}1)$		
4	$[111](1\bar{2}1)$		
5	$[111](\bar{2}11)$		

The incoherent crystal structure of cementite layer acts as a barrier to dislocation transmission, which in turn develops stress concentration in cementite layer. Thus, in P1, the developed stress is high enough to deform the thin cementite layer and nucleates new dislocation loops in the bottom layer of ferrite. In contrast, in P3 and P5 samples, dislocations were not formed below the cementite layer due to smaller compliance of thicker cementite layers to transmit stress to bottom ferrite layer.

Figure 4. Dislocations evolution after 30 Å indentation of indenter with 5 nm radius in pure Fe, P1, P3 and P5 samples at (a) 100 K, (b) 300 K and (c) 700 K. Atoms on a perfect BCC lattice were not visualized. Cementite layers are illustrated by black arrows.

Figure 5. Dislocations evolution after 30 Å indentation of indenter with 7 nm radius in pure Fe, P1, P3 and P5 samples at (a) 100 K, (b) 300 K and (c) 700 K. Dislocations are formed in the bottom ferrite layer in all deformed samples. Atoms on a perfect BCC lattice were not visualized. Cementite layers are illustrated by black arrows.

In order to investigate the effect of indenter radius on dislocation evolution during nanoindentation, additional simulation tests were performed with 5 and 7 nm indenter radius. Figures 4 and 5 illustrate the dislocation structure at different temperatures of 100, 300 and 700 K in nanocomposite samples after 30 Å indentation by indenters with 5 and 7 nm radius, respectively. We found higher dislocation activity in pure Fe sample when the indenter radius increases. **Beyond the yield point, the volume occupied by the indenter causes the permanent deformation which should be accommodated by geometrically necessary dislocations (GNDs).** The volume occupied by the indenter with 3, 5 and 7 nm radius at 30 Å indentation depth is 18π , 36π and 54π nm³, respectively. Hence, the larger indenter generates higher GND density at the same indentation depth. In other words, larger indenter radius induces higher stress on the cementite layer, which leads to dislocation nucleation below the thicker cementite layer. However, we find that no dislocation loops are formed in the bottom ferrite layer of P5 sample regardless of imposed temperatures during indentation by indenter with 5 nm radius, while the 7 nm radius indenter generates new dislocations below the cementite layer in all nanocomposite samples and at all temperatures. Thus, we can conclude that the dislocation blocking capability increases with the thickness of the cementite.

Comparison of Figures 3, 4 and 5 reveal the effect of temperature on the dislocation activity in the ferrite part. It is interesting to note that the dislocation nucleation in bottom ferrite layer decreases as temperature rises, while the activation of new slip systems are more facile in the ferrite at elevate temperature [35]. As temperature rises, the dislocations in top ferrite part (or pure Fe sample) become more distributed, and more frequently annihilate with each other. This implies that the cementite layer

experiences less stress concentration, implying smaller chance for dislocation nucleation in the bottom ferrite layer. The onset of dislocation nucleation in the bottom ferrite layer is associated with load drop that is marked by gray arrows in Figure 2 (c) for indenters with 5 nm and 7 nm radii. Unfortunately, it is impossible to identify the dislocation nucleation in the bottom ferrite layer merely from load-displacement curves, because the plastic response from cementite layer is overlapped. Indeed, the curve for 3 nm radius case, which does not experience the dislocation nucleation in the bottom ferrite, looks qualitatively similar to others.

To further investigate the deformation mechanisms in detail, an atomic shear strain analysis was performed following the approach by Shimizu et al. [26]. Figure 6 presents the atoms with shear strain more than 0.1 in deformed samples at 30 Å indentation depth by 3 nm radius indenter at different temperatures. In pure Fe sample, shear strain spread laterally at 100 K, and increasing temperature causes more depth-wise spreading of the strained region. However, due to the existence of cementite layer, different deformation behavior is observed in P1, P3 and P5 samples, where lateral spreading of the strained region is more pronounced at elevated temperature as shown in Fig. 6(b)-(c).

Figures 7 and 8 also represent the shear strain distribution in deformed sample by indenter with 5 and 7 nm radius, respectively. Comparison of shear strain distribution in Figures 6, 7 and 8 reveals the effect of indenter radius on the strain distribution in cementite layer. While the shear strain is almost trapped by the cementite layer in figure 6 (3 nm indenter radius), the strained region spreads below the thicker cementite layer in more samples when indenter radius increases in figure 7 and 8 due to higher dislocation activities.

Figure 6. Atomic shear strain distribution of Fe and C atoms after 30 Å indentation of 3 nm indenter radius at (a) 100 K, (b) 300 K and (c) 700 K. Only atoms with shear strain more than 0.1 have been showed. Dashed lines illustrate cementite layers and red color points indicate the atoms with a shear strain equal or more than 1.

Figure 7. Atomic shear strain distribution of Fe and C atoms after 30 Å indentation of 5 nm indenter radius at (a) 100 K, (b) 300 K and (c) 700 K. Only atoms with shear strain more than 0.1 have been showed.

Figure 8. Atomic shear strain distribution of Fe and C atoms after 30 Å indentation of 7 nm indenter radius at (a) 100 K, (b) 300 K and (c) 700 K. Only atoms with shear strain more than 0.1 have been showed.

In order to clarify the deformation mechanism in nanocomposite pearlite structure, we count the fraction of highly strained atoms in deformed samples. Figure 9(a) shows the effect of temperature on the percent of atoms with shear strain more than 0.1 in deformed samples after indentation of 30 Å by indenter with 5 nm radius. As temperature rises, the percent of high strained atoms increases gradually for all deformed samples, implying more distributed deformation at elevated temperature. Same behavior was observed for other indenter radiuses.

On the other hand, Figure 9(b) reveals the effect of indenter radius on the percent of high strained atoms. An increase in indenter radius in Figure 9(b) increases the percent of high strained

atoms dramatically, due to higher density of GNDs. However, we find in Figure 9(c) that the increasing cementite thickness significantly decreases the percent of high strained atoms for all indenter radii at a constant temperature. In other words, thicker cementite layer is more effective in trapping dislocation propagation and act as an obstacle for preventing plastic deformation of the bottom ferrite layer. In contrast, at lower temperature, thinner cementite layer is less likely to sustain the localized stress by the dislocation pile-up at the interface during the indentation.

Figure 9. Percent of atoms with shear strain more than 0.1 in deformed samples; (a) temperature effect, (b) indenter radius effect and (c) cementite thickness effect. The indenter radius in (a) is 5 nm and the temperature in (b) and (c) is 100 and 700 K, respectively.

4. Conclusions

In this work, we performed molecular dynamics simulations of the nanoindentation test to investigate the role of cementite in blocking dislocation propagation in pearlite structure. The load-displacement curves were found to change with temperature mainly in plastic region and the presence of cementite layer does not affect the elastic response significantly. However, the indentation load rises significantly with larger indenter radius size. We find that the cementite layer acts as a hard obstacle to dislocation propagation in pearlite. We also show that increasing temperature enhances the distribution of plastic strain in the ferrite layer, which reduces the stress acting on the cementite layer. Thus, we find that the dislocation propagation is more likely to form for a thin cementite layer at low temperature with large indenter radius.

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Appendix A. Generalized stacking fault energy of (010) plane in cementite:

In order to test the ability of MEAM empirical potential to reproduce plasticity, dislocations, and the slip system of the cementite, we calculated generalized stacking fault (GSF) energy of the (010) plane in cementite and compared with the *ab initio* results. The (010) planes are grouped into two types; one type is a plane between two neighboring layers of only Fe atoms (labeled as type I hereinafter) while the other is the one between Fe and Fe/C layers (labeled as type II). The stacking fault (SF)

energy along the [100] and [001] directions on both types of (010) planes was calculated by introducing relative slip across the slip plane in the crystal and accomplishing relaxation at $T=0$ K as introduced in [36]. For *ab initio* calculations, we used the Vienna *ab initio* simulation package (VASP) [37] with the local density approximation (LDA). A simulation cell of $[100] \times 3[010] \times [001]$ containing 48 atoms (36 Fe atoms and 12 C atoms) was employed under periodic boundary conditions imposed along [100] and [001]. The k -points are sampled by a $4 \times 1 \times 4$ Monkhorst-Pack method and the cut-off energy for the plane wave is 38.22 Ry. The results of molecular statics (MS) and *ab initio* simulation are shown in Fig. A.1. Every local minimum in Fig. A.1(a) indicates formation of a partial dislocation along the [100] in (010) slip planes in cementite. Both MS and *ab initio* agree that partial formation is more preferable in type I plane or a plane between only Fe-atom layers. On the other hand, in Fig. A.1(b), no local minima is observed along the [001] direction on type II cross section in both MS and *ab initio*. A plateau region is predicted on type I cross section by both MS and *ab initio*, and the *ab initio* curve has wider plateau with small local minima. However, at finite temperature, the effect of such a small minima would be negligible. Overall, the MEAM potential captures the characteristic features in GSF curves qualitatively well, and is considered as a reliable model to simulate plastic event in cementite. Stable stacking fault energy and the corresponding displacement are summarized in Table A.1.

Besides, our results are consistent with experimental observation, where the embedded cementite particles in ferrite matrix are deformed through the movement of stacking faults, which characterized by an $\alpha[100](010)$ partial dislocation [35,38]. The GSF energy of (010) cementite slip plane was also calculated using *ab initio* method. Our results are also consistent with *ab initio* results, where the local minima only observed along [100] direction on both cross section of (010) cementite plane.

Table A.1. Stable stacking fault energy γ and corresponding displacement Δx in the (010)[100]

slip system. In MEAM MS, the lattice constants are $a = 5.05$, $b=6.69$, and $c=4.49$ ($\text{\AA}$) and those in ab initio are $a = 4.926$, $b = 6.623$, $c = 4.377$ ($\text{\AA}$).

	MEAM MS		Ab initio	
	$\gamma(\text{eV}/\text{\AA}^2)$	Δx	$\gamma(\text{eV}/\text{\AA}^2)$	Δx
Section I	0.079	0.4[100]	0.059	0.3[100]
Section II	0.096	0.49[100]	0.082	0.3[100]

Figure A.1. Stacking fault energy of (010) plane along (a) [100] and (b) [001] directions with different types of cross section. Circles and triangles indicate MS results and ab initio results, respectively. The

local minima indicate favorable displacement of atoms.

Appendix B. Calculation of elastic moduli of ferrite and cementite

In order to obtain the Young's moduli of ferrite and cementite, we calculated the elastic constants of ferrite and cementite at 100 K, 300 K and 700 K using Liyanage's MEAM potential [22]. The each component of elastic modulus tensor was computed from the stress-strain curves obtained by MD simulations at a given temperature in the NVT ensemble. Due to the complex screening function of the MEAM potential used in this study, elastic softening was observed only at the temperatures higher than 300 K. Such anomaly in elastic response would not have a considerable effect on the plastic response observed in this study.

$$C_{f-100K} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix} = \begin{bmatrix} 220 & 147 & 147 & 0 & 0 & 0 \\ 147 & 220 & 147 & 0 & 0 & 0 \\ 147 & 147 & 220 & 0 & 0 & 0 \\ 0 & 0 & 0 & 126 & 0 & 0 \\ 0 & 0 & 0 & 0 & 126 & 0 \\ 0 & 0 & 0 & 0 & 0 & 126 \end{bmatrix} \quad (B.1)$$

$$C_{c-100K} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{22} & c_{23} & 0 & 0 & 0 \\ c_{13} & c_{23} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix} = \begin{bmatrix} 306 & 141 & 164 & 0 & 0 & 0 \\ 141 & 234 & 119 & 0 & 0 & 0 \\ 164 & 119 & 322 & 0 & 0 & 0 \\ 0 & 0 & 0 & 22 & 0 & 0 \\ 0 & 0 & 0 & 0 & 99 & 0 \\ 0 & 0 & 0 & 0 & 0 & 66 \end{bmatrix} \quad (B.2)$$

$$C_{f-300K} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix} = \begin{bmatrix} 222 & 145 & 145 & 0 & 0 & 0 \\ 145 & 222 & 145 & 0 & 0 & 0 \\ 145 & 145 & 222 & 0 & 0 & 0 \\ 0 & 0 & 0 & 127 & 0 & 0 \\ 0 & 0 & 0 & 0 & 127 & 0 \\ 0 & 0 & 0 & 0 & 0 & 127 \end{bmatrix} \quad (B.3)$$

$$C_{c-300K} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{22} & c_{23} & 0 & 0 & 0 \\ c_{13} & c_{23} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix} = \begin{bmatrix} 288 & 146 & 158 & 0 & 0 & 0 \\ 146 & 248 & 120 & 0 & 0 & 0 \\ 158 & 120 & 309 & 0 & 0 & 0 \\ 0 & 0 & 0 & 33 & 0 & 0 \\ 0 & 0 & 0 & 0 & 93 & 0 \\ 0 & 0 & 0 & 0 & 0 & 79 \end{bmatrix} \quad (B.4)$$

$$C_{f-700K} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix} = \begin{bmatrix} 214 & 136 & 136 & 0 & 0 & 0 \\ 136 & 214 & 136 & 0 & 0 & 0 \\ 136 & 136 & 214 & 0 & 0 & 0 \\ 0 & 0 & 0 & 126 & 0 & 0 \\ 0 & 0 & 0 & 0 & 126 & 0 \\ 0 & 0 & 0 & 0 & 0 & 126 \end{bmatrix} \quad (B.5)$$

$$C_{c-700K} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{22} & c_{23} & 0 & 0 & 0 \\ c_{13} & c_{23} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix} = \begin{bmatrix} 258 & 147 & 147 & 0 & 0 & 0 \\ 147 & 241 & 118 & 0 & 0 & 0 \\ 147 & 118 & 281 & 0 & 0 & 0 \\ 0 & 0 & 0 & 33 & 0 & 0 \\ 0 & 0 & 0 & 0 & 83 & 0 \\ 0 & 0 & 0 & 0 & 0 & 72 \end{bmatrix} \quad (B.6)$$

Ferrite and cementite have body centered cubic (BCC) and orthorhombic structures, respectively. For arbitrary loading direction, the Young's moduli in the cubic and orthorhombic symmetry crystals are given by the following equations, respectively [39]:

$$1/E_{ferrite} = S_{11} + [S_{44} - 2(S_{11} - S_{12})](a_{11}^2 a_{12}^2 + a_{12}^2 a_{13}^2 + a_{13}^2 a_{11}^2) \quad (B.7)$$

$$1/E_{cementite} = S_{11}a_{11}^4 + S_{22}a_{12}^4 + S_{33}a_{13}^4 + a_{11}^2 a_{12}^2 (2S_{12} + S_{66}) + a_{11}^2 a_{13}^2 (2S_{13} + S_{55}) + a_{12}^2 a_{13}^2 (2S_{23} + S_{44}) \quad (B.8)$$

where, E is Young's modulus, S_{ij} are compliance elastic constants ($\mathbf{S}=\mathbf{C}^{-1}$), and a_{li} are direction cosines of the arbitrary tensile direction represented in the symmetry axes. Table B.1 shows the calculated Young's moduli of ferrite and cementite along $[11\bar{2}]_f$ and $[010]_c$ at 100, 300 and 700 K:

Table B.1. Calculated Young's moduli of ferrite and cementite along $[11\bar{2}]_f$ and $[010]_c$ at 100, 300 and 700 K.

Temperature (K)	$E_{ferrite}$ along $[11\bar{2}]_f$ (GPa)	$E_{cementite}$ along $[010]$ (GPa)
100	203	159
300	209	158
700	208	154

The effective elastic moduli can also be obtained from Ruess model for P0, P1, P3 and P5 samples:

Table B.2. The effective Young's moduli of P0, P1, P3 and P5 samples along y direction at 100, 300 and 700 K.

Sample Name	Elastic modulus at 100 K (GPa)	Elastic modulus at 300 K (GPa)	Elastic modulus at 700 K (GPa)
P0	203	209	208
P1	198	203	202
P3	192	196	194

P5	188	191	188
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