

Atomistic modeling of plastic deformation in B2-FeAl/Al nanolayered composites

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Abstracts

In this work, the deformation response of the B2-FeAl/Al intermetallic composites, as a model material system for nanolayered composites comprised of intermetallic interfaces, has been explored. We use atomistic simulations to study the deformation mechanisms and the interface misfit dislocation structure of B2-FeAl/Al nanolayered composites. It is shown that two sets of dislocations are contained in the interface misfit dislocation network and are correlated with the initial dislocation nucleation from the interfaces. The effects of layer thickness on the uniaxial deformation response of the B2-FeAl/Al multilayers are investigated. We observed that under compressive loading the smaller proportion of the FeAl layers leads to the lower overall flow stress. Under tensile loading, the void formation mechanism is investigated, suggesting the interface structure and the dislocation activities in the FeAl layers playing a significant role to trigger the strain localization which leads to void nucleation commencing at the interface. It is also found that the deformation behavior in the “weak” Fe/Cu interface behaves substantially different than that of the “strong” FeAl/Al interface. The atomistic modeling study of the nanolayered composites here underpinned the mechanical response of “strong” intermetallic interface material systems. There is no void nucleation during the entire plastic deformations in the Fe/Cu simulations, which is attributed to much higher dislocation density, more slip systems activated, and relative uniformly distributed dislocation traces in the Fe phase of the Fe/Cu multilayers.

Keywords: Nanolayered composites; Intermetallic; Plastic deformations; Dislocations

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1. Introduction

High fraction of interfacial content and local interface structures in the nanolayered composites play a significant role in their mechanical responses [1-7]. Interfaces can serve as the crucial sources of plasticity carrier, barrier for dislocation movement, sinks for dislocations through annihilation and absorption, and storage sites for defects [8-15]. Three main kinds of interfaces are included in the nanolayered composites: coherent, semi-coherent, and incoherent interfaces [16-20]. For relatively small misfits between the two phases, the interface boundary forms a semi-coherent interface. The dislocation content of the semi-coherent interfaces can often be described by the interface misfit dislocation network [21-24].

Due to the importance of the topic, there have been many studies in literature, both in experimental and modeling works in bi-metallic interfaces. A particular aspect in these studies is focused on the role of dislocations played during the mechanical response of nanolaminates. Dislocations can easily move between two layers in coherent interfaces since the slip systems are nearly continuous [8]. In incoherent interfaces, dislocation slip systems in the two adjacent layers are not continuous because of the large difference in lattice structures or large lattice mismatch, which may cause occurrence of the interface shearing [21,25]. For semi-coherent interfaces, there is length-dependent behavior [26]. For layer thickness from microns to tens of nanometers, there is strength increase with the decrease of individual layer thickness involving dislocation pile-ups (Hall-Petch strengthening). When the layer thickness decreases to a certain small value about 2-5 nm, the strength of metallic nanolayered composites has a maximum value, which was explained by a single dislocation crossing interfaces [1,27,28]. The deformation responses including the properties of interfaces of metallic nanolayered composites have also been explored in various studies under different loading conditions [29-33,26,34]. For example, Abdolrahim et al. [16] using molecular dynamics (MD) simulations to explore the influence of the layer thickness of Cu-Nb multilayers on deformation mechanisms under biaxial tensions. It was concluded that the transitions from Hall-Petch strengthening to dislocation confined layer slip to dislocation nucleation, control the deformation responses corresponding to length scale from microns to few tens of nanometers to less than few nanometers. Yadav et al. [35] demonstrated that the interface shear mechanism of Mg/Nb is anisotropic and related to shear loading directions. More recently, our MD simulation results show good agreement with experimental results that the inverse size effect in the strength occurs in samples with layer thickness below 2.0 nm [5]. The quantitative

analysis revealed that the unsymmetrical dislocation transmission across the interface induces the shear localization and promotes the shear band formation in Cu/Nb nanolaminates. The plastic strain primarily comes from the interface sliding within the shear band.

However, there have been very few studies on the nanolayered composites comprised of intermetallic interfaces and their deformation responses. Recently, Choudhuri et al. [36,37] used MD simulations to study the effect of interfaces of the Ni/NiAl intermetallic composites on uniaxial deformation mechanisms, which depends on the B2-NiAl layer thickness. In another MD simulation study, it is found that in nanoscale composites Al-Al₂Cu, plasticity is accommodated by localized shear on unusual slip planes, which is because of the continuity of slip systems across the interfaces [38]. A further systematic atomistic modeling study on the nanolayered composites comprised of intermetallic interfaces and their deformation responses will help to better understand the mechanical response of such material systems.

In this paper, we explore the deformation response of the B2-FeAl/Al intermetallic composites. We choose B2-FeAl/Al as a model material system for nanolayered composites comprised of intermetallic interfaces. B2-FeAl is also considered to be an unusually ductile intermetallic phase and the dislocation behavior in this B2 alloy is well studied [39], thus making this nanolaminate system especially attractive to be studied. Fe/Al multilayers have also been experimentally studied before [40]. Under annealing conditions, the intermetallic phase FeAl can form. In this study, the Frank-Bilby (F-B) equation analysis is firstly used to investigate the interface misfit dislocation content of the B2-FeAl/Al interface. MD simulations are then carried out to study the compression and tension deformation mechanisms under uniaxial loading conditions. In addition, the void and crack formation mechanisms which occurred during the MD simulations are analyzed. Finally, to further determine the relationship between void nucleation mechanism and interface properties, a comparative study of the Fe/Cu interface was also carried out in this paper.

2. Methods

The plastic deformation simulations of the B2-FeAl/Al lamellar metallic nanocomposites were investigated using the large-scale atomic/molecular massively parallel simulator (LAMMPS) program [41]. For Fe-Al, the interatomic potential employed is the Finnis–Sinclair (FS) potential

developed by Mendelev et al. [42]. This potential was fitted to DO₃ and L1₂ Al₃Fe intermetallic phases. In addition, it has been used successfully before to study the core structures and planar faults of dislocations in B2-FeAl intermetallic [43]. For Fe-Cu, the embedded atom method (EAM) potential developed by Bonny et al. [44] was employed. In Table 1, some relevant basic properties were calculated from the above empirical potentials, such as the stacking fault energies of Al, Cu, vacancy formation energy of Fe, the relative energy of Fe bcc phase relative to the fcc phase, and the formation energy of B2-FeAl are listed. These values are compared to available experimental data and the first-principles density functional theory (DFT) based calculations if experimental data is not available or has large uncertainty. From Table 1, it is seen that the values calculated using empirical potential have good agreement with experiments or DFT values.

The Kurdjumov-Sachs (KS₁) orientation relationship for the B2-FeAl/Al interface was set up such that (111)_{Al}|| (110)_{FeAl} and (110)_{Al}|| (111)_{FeAl} [45,46]. The unit cells of fcc-Al and B2-FeAl are respectively shown in figures 1a and 1b. The B2-FeAl/Al multilayers configuration with 5 nm layer thickness is shown in figure 1c, with the *x* direction along [11 $\bar{2}$]_{Al}//[1 $\bar{1}$ 2]_{FeAl}, the *y* direction along [1 $\bar{1}$ 0]_{Al}/[$\bar{1}$ 11]_{FeAl}, and the *z* direction along [111]_{Al}//[110]_{FeAl}. The *z* direction is perpendicular to the interface. The dimensions of the simulation box are about 33.7 nm in the *x* direction and 44.6 nm in the *y* direction. The dimension in the *z* direction is varied with the layer thickness. The number of atoms in the simulations ranges from 994560 to 3632200.

The relaxation of simulation supercells was accomplished by using the conjugate gradient method, followed by the isothermal-isobaric (NPT) ensemble over 200 ps to reach their most stable configurations. The periodic boundary conditions (PBC) were utilized along *x*, *y* and *z* directions to keep the repeatability of the simulation box. Uniaxial compressive loading normal to the interface plane and uniaxial tensile loading parallel to the interface were applied to the simulation models at a constant strain rate of 3 x 10⁸/s. The crystallography of the simulation model was visualized using the common neighbor analysis (CNA) algorithm [47]. The dislocation characteristic was identified using the dislocation extraction algorithm (DXA) [48] as implemented in OVITO software [49]. For disregistry analysis, disregistry vectors $\Delta\vec{r}$ was computed as,

$$\Delta\vec{r} = \vec{r}_{ij}^{int} - \vec{r}_{ij}^{ref} \quad (1)$$

Where $\vec{r}_{ij}^{ref}$ is the relative position between the i th atom and the j th atom that form a pair in the reference configuration and $\vec{r}_{ij}^{int}$ is the relative position between the same pair of atoms at the interface [50-52].

To make a quantitative analysis of the interface misfit dislocation content in the B2-FeAl/Al interface, the Frank-Bilby (F-B) equation analysis [21,53-55] was carried out. The F-B equation analysis quantifies the total Burgers vector $\vec{B}$ intercepted by a probe vector $\vec{v}$ in an interface of interest,

$$\vec{B} = (\mathbf{A}_P - \mathbf{A}_Q) \vec{v} \quad (2)$$

Where, $\mathbf{A}_{P,Q}$ is the transformation matrix that transforms crystal lattice P/Q into a reference state by an affine deformation. P and Q are the crystal phases in the bi-crystal with the interface. This is equivalent to the following (see appendix D of Hirth et al [21]),

$$\sum \frac{\vec{b}_i \sin \gamma_i}{d_i} = \mathbf{D}_{rc} \vec{p}, \quad (3)$$

where each set of dislocations with Burgers vectors $\vec{b}_i$ consists of a parallel array with spacing d_i , γ_i is the angle between $\vec{v}$ and the line direction of the i th set, $\vec{p}$ is a unit probe vector parallel to $\vec{v}$, and the sum is over all sets of misfit dislocations. $\mathbf{D}_{rc}$ represents a deformation matrix that maps a unit vector in the rotated coherent reference configuration into the natural interface that contains the interface misfit dislocations. This method has been successfully applied to a number of different interfaces, e.g., Al/Al₂O₃ interface [52], Al/Si interface [56], SrTiO₃/MgO interface [57], etc..

3. Results

3.1 Interface misfit dislocation content of the KS FeAl/Al interface

In figure 2, the atomic structure of the constructed KS interface after atomic relaxation is shown. In order to apply the F-B equation analysis, the reference structure was taken as the rotated coherent dichromatic pattern (RCDP) in the topological theory [21]. The basis vectors in fcc-Al and B2-FeAl lattices at the interface plane are represented by $\mathbf{M}$,

$$\mathbf{M}_{Al} = [\vec{v}_{Al}^1, \vec{v}_{Al}^2] \quad (4)$$

$$\mathbf{M}_{FeAl} = [\vec{v}_{FeAl}^1, \vec{v}_{FeAl}^2] \quad (5)$$

where $\vec{v}_{Al}^1 = \begin{bmatrix} 0 \\ a_{Al}/\sqrt{2} \end{bmatrix}$, $\vec{v}_{Al}^2 = \begin{bmatrix} -a_{Al}\sqrt{3}/(2\sqrt{2}) \\ a_{Al}/(2\sqrt{2}) \end{bmatrix}$; and $\vec{v}_{FeAl}^1 = \begin{bmatrix} 0 \\ a_{FeAl}\sqrt{3}/2 \end{bmatrix}$, $\vec{v}_{FeAl}^2 = \begin{bmatrix} -a_{FeAl}\sqrt{6}/3 \\ a_{FeAl}\sqrt{3}/6 \end{bmatrix}$; with a_{Al} and a_{FeAl} are the lattice constant of Al (4.0333 Å) and FeAl (2.8513 Å), respectively. The distortion matrix (or the strain matrix) required to be applied to either Al or FeAl to obtain the RCDP reference are,

$${}_{rc}\mathbf{D}_{Al} = -0.5(\mathbf{M}_{Al} - \mathbf{M}_{FeAl})\mathbf{M}_{Al}^{-1} = \begin{bmatrix} -0.0287 & 0.0 \\ 0.0833 & -0.067 \end{bmatrix} \quad (6)$$

$${}_{rc}\mathbf{D}_{FeAl} = 0.5(\mathbf{M}_{Al} - \mathbf{M}_{FeAl})\mathbf{M}_{FeAl}^{-1} = \begin{bmatrix} 0.031 & 0.0 \\ -0.102 & -0.078 \end{bmatrix} \quad (7)$$

As a sanity of check, $({}_{rc}\mathbf{D}_{Al} + \mathbf{I})\mathbf{M}_{Al} = ({}_{rc}\mathbf{D}_{FeAl} + \mathbf{I})\mathbf{M}_{FeAl}$, both reaching the RCDP reference.

The disregistry plot for the relaxed KS interface using the unrelaxed KS interface as the reference is shown in figure 3. From figure 3, it is suggested that two sets of misfit dislocations may constitute the interface misfit dislocation network, which can be conveniently called *Set-1* and *Set-2* dislocations. *Set-1* dislocations are vertically lined. *Set-2* dislocations have an angle θ of 56.5° relative to the vertical line. ${}_n\mathbf{D}_{rc}$ represents a deformation matrix that maps a unit vector in the RCDP configuration into the natural interface structure containing dislocations,

$${}_n\mathbf{D}_{rc} = ({}_{rc}\mathbf{D}_{Al} + \mathbf{I})^{-1} - ({}_{rc}\mathbf{D}_{FeAl} + \mathbf{I})^{-1} = \begin{bmatrix} 0.059 & 0.0 \\ -0.184 & 0.144 \end{bmatrix} \quad (8)$$

Since there are two sets of dislocations, one can choose to use probe vector $\vec{p}$ to be parallel to the line direction of one set of the dislocations. In case 1, the probe vector was chosen to be $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$, which is parallel to the line direction of *Set-1* dislocations. Applying this to the F-B equation (Eq. (3)), the information regarding *Set-2* dislocations was obtained,

$$\frac{\vec{b}_2}{d_2} = \begin{bmatrix} 0.0 \\ 0.144 \end{bmatrix} \quad (9)$$

This led to $\vec{b}_2 = (0, 2.66 \text{ \AA})$ with a dislocation spacing of 15.45 Å. This Burgers vector has an edge component of 2.22 Å and a screw component of 1.47 Å. In case 2, the probe vector is chosen to be in parallel to the line direction of *Set-2* dislocations. Applying this to the F-B equation, the information regarding *Set-1* dislocations was obtained,

$$\frac{\vec{b}_1 \sin(\theta)}{d_1} = \begin{bmatrix} 0.059 \sin(\theta) \\ -0.184 \sin(\theta) + 0.144 \cos(\theta) \end{bmatrix} \quad (10)$$

where θ is the angle between the probe vector and the z axis (56.5°). This led to $\vec{b}_1 = (2.48 \text{ \AA}, -3.72 \text{ \AA})$ with a dislocation spacing of 41.95 Å. This Burgers vector is rather large, of 4.46 Å in length, with edge component 2.48 Å and screw component of -3.72 Å. In figure 3, these two sets of dislocations as the interface misfit dislocation content are also shown.

This is the first time that F-B equation analysis is used to characterize the interface misfit dislocation network at the FeAl/Al KS interface. From such analysis, two sets of dislocations as the interface misfit dislocation content at the interface were identified, with one set of dislocation with strong core-overlap and mainly of edge type character while the other set of dislocations in distant distance away from each other and more of screw type character.

3.2. B2-FeAl/Al deformations

3.2.1 Dislocation nucleation from the FeAl/Al interface

Dislocation nucleation commences at the interface from the softer Al phase during early plastic deformations. Figure 4 shows the dislocation nucleation process at the interface in the Al phase. To clearly visualize the dislocation networks, the perfect fcc and bcc atoms have been removed. Compared with the misfit interfacial dislocation network in Section 3.1, the dislocation nucleation sites at the interface are mainly along the set of dislocation $\vec{b}_1$ lines with the same dislocation spacing, and the Burgers vectors of the nucleated dislocations are different. The Burgers vectors of dislocations nucleated from the interface in the Al phase are primarily $1/6[1\bar{1}2]$. The Schmid factor for the activated slip system of $1/6[1\bar{1}2]$ ($1\bar{1}\bar{1}$) is 0.1571 when the simulation box is subjected to the loading normal to interface. Both the interface structure and the Schmid factor could affect dislocation nucleation from interfaces, according to Ref. [32]. The activated slip system has a positive large Schmid factor and is distributed along the misfit dislocation line,

which was observed similarly in MD simulations with Cu/Nb composites [12]. Of the nucleated dislocations, some dislocations propagate in the form of two Shockley partials $1/6\langle 112 \rangle$ (yellow lines in figure 4) and stair-rod dislocation $1/6\langle 110 \rangle$ (pink lines in figure 4) and expand into the Al layers. The Shockley partials nucleated from the interface will contribute to the subsequent dislocation activities at the interface while the stair-rod dislocation will not due to its sessile nature.

3.2.2 Deformation response under compressive loading normal to the interface

Uniaxial compressive loading normal to the interface was applied to the B2-FeAl/Al simulation models. To investigate the effect of the layer thickness on plastic deformation, the structures with two different ratios of the layer thickness of B2-FeAl to that of Al were studied. This results in a total of four simulation models: FeAl-2nm/Al-2nm, FeAl-5nm/Al-5nm, FeAl-2nm/Al-4nm, and FeAl-5nm/Al-10nm, each representing thickness of 2 nm, 5 nm, 2 nm (FeAl)/4 nm (Al), and 5 nm (FeAl)/10 nm (Al) in the nanocomposite samples.

The compressive stress-strain curves during the MD simulations are shown in figure 5a and the simulation supercells were deformed up to 25% strain. The results indicate that the structures with B2-FeAl to Al layer thickness ratio of 1:1 have a higher peak stress than the structures with the thickness ratio of 1:2. This is mainly due to the higher elastic modulus of B2-FeAl compared to that of Al. After about 18% applied strain, all stress-strain curves exhibit decreasing trend with the increasing applied strain. Furthermore, a rapid decrease in the stress-strain curves of multilayers with FeAl in 2 nm thickness was observed. In comparison, the multilayers with FeAl in 5nm thickness experience a more gradual stress reduction. The mechanical responses at different layer thickness ratios, with the average flow stress calculated from 10% to 20% strain, are compared in figure 5b. The structures with the thickness ratio of 1:1 have a higher average flow stress, which indicates that the higher B2-FeAl fraction leads to the strengthening of the nanocomposites. It suggests that decreasing the ratio of the B2-FeAl thickness relative to the Al phase will reduce the overall flow stress. Note that the difference of average flow strength of structures Al-2nm/FeAl-2nm and Al-5nm/FeAl-5nm is very small. To explain the small difference in strength, further simulations of structures Al-3.4nm/FeAl-3.4nm and Al-8nm/FeAl-8nm were carried out. The result suggests that average flow strength and layer thickness satisfy

the inverse Hall-Petch relationship under small layer thickness (about 3.4 nm), i.e., strengthening from 8 nm to 3.4 nm, and softening from 3.4 nm to 2 nm.

Plastic deformation responses of the nanolaminates studied are assumed to be mostly through the dislocation activities under loading conditions. Hence, the dislocation density evolution during mechanical loadings is quantitatively collected. A comparison of such dislocation density for different types of dislocations observed during MD simulations of the FeAl-5nm/Al-5nm multilayers is shown in figures 6a (in Al layers) and 6b (in FeAl layers), which investigates the evolution of different Burgers vectors as a function of compressive strain. We chose this particular sample due to its typical behavior representing all other samples studied. The dislocation density is calculated using the total length of dislocation lines in each layer divided by its simulation cell volume. Results show that dislocations initiate in the Al layers at strain about 5.85% and dislocations nucleate in the FeAl layers at a larger strain level, about 7.2%. The dislocation density in the Al layers is substantially larger than that in the FeAl layers. Figure 6a shows that the dislocation density of $1/6\langle 112 \rangle$ partials surpass the perfect $1/2\langle 110 \rangle$ and stair-rod $1/6\langle 110 \rangle$ dislocations by nearly an order of magnitude in the Al layers. Thus, the Shockley partial dislocation of $1/6\langle 112 \rangle$ seems to primarily affect the plasticity in the Al layer. Figure 6b shows that inside the FeAl layers, the dislocation density with Burgers vector of $1/2\langle 111 \rangle$ is larger than that with $\langle 100 \rangle$.

To better understand the compressive response of the B2-FeAl/Al composites, we have also investigated the evolution of atomic configurations with compressive strains. The result is shown in figure 7 for the FeAl-2nm/Al-2nm sample. Figure 7a-f show the deformation evolution with several strains at 22.5%, 24%, and 25.5%, respectively. In figure 7a-b, it is noted that the local B2 structure in the FeAl layer is converted to fcc-like structure (a mixture of fcc + hcp layers), which is consistent with previous study relating to fcc-B2 nanostructures [36]. Earlier experimental works suggested that under irradiation conditions, FeAl could be phase transformed to $L1_0$ phase (CuAu $L1_0$ structure, which is a tetragonal distortion of the fcc structure), with chemical disorders [58]. In larger sized samples, such phase transformation did not occur.

As the strain increases, the sheared deformation is observed in the local FeAl and the adjacent Al layers in figure 7c and 7f. This explains the relatively faster stress decrease in the stress-strain curves of the FeAl-2nm multilayers. Figure 7d-f also show that the local shear strain

accumulation is primarily associated with dislocation activities and sheared regions. The sheared deformation is prompted by the phase transformation in the newly formed fcc-like structure in the FeAl layer.

The main findings from the MD simulations of the deformation response of the FeAl/Al multilayers under compression loading normal to the interface are in the following. Firstly, stress-strain curves suggest the effect of individual layer thickness on flow strength and the smaller proportion of the FeAl layers leads to the overall lower flow stress. This is in general agreement with other similar simulations of hard/soft combinations of multilayers. Secondly, the dislocations of Shockley partials in fcc and dislocations of $\frac{1}{2}\langle 111 \rangle$ in B2 structures are the dislocations that primarily accommodate the plastic deformation. The dominance of Shockley partials in fcc phase was also observed in a recent study of the deformation studies of B2-NiAl/Ni multilayers [37]. However, in that study, it was observed that the amount of $\frac{1}{2}\langle 111 \rangle$ dislocations is comparable to that of $\langle 100 \rangle$ dislocations in the B2 phase. Such detailed analysis of dislocation activity could provide a useful information for mesoscale dislocation dynamics simulations. Thirdly, in the multilayers with thin layer thickness of 2 nm FeAl, shearing deformation is observed, prompted by the phase transformation in fcc-like region converted from the B2 structure. This particular phenomenon only occurred at small individual layer thickness (2 nm) sample and was not observed in larger samples. This is observed for the first time for the intermetallic based multilayers. In earlier studies, at smaller layer thicknesses, 5 nm or below, micropillar investigation revealed the evidence of co-deformation in both the Al and TiN phases in TiN/Al multilayers [59,60], it seems though, that this co-deformation may not be applicable to the B2-FeAl/Al multilayers.

3.2.3 Deformation response under tensile loading parallel to the interface

In figure 8, the typical tensile loading stress-strain curves of the B2-FeAl/Al composites in two different B2-FeAl to Al layer thickness ratios of 1:1 and 1:2 are shown. We performed four MD simulations in total, for FeAl-2nm/Al-2nm, FeAl-5nm/Al-5nm, FeAl-2nm/Al-4nm, and FeAl-5nm/Al-10nm, with tensile loadings under the x direction (along $[11\bar{2}]_{\text{Al}}/[1\bar{1}2]_{\text{FeAl}}$). For simulations of larger FeAl thickness samples (5 nm), stress fluctuates at around 3 GPa before applied strain of 15% and then gradually decreases. While for simulations of smaller FeAl thickness samples (2 nm), stress experiences a more abrupt large drop down to nearly zero after the peak value. This is due to rapid void and crack formation during the simulations. The nanolaminates

with the thickness ratio of 1:1 has a significant higher peak stress than that of the structure with the thickness ratio of 1:2, similar to what observed in the compressive loading case above. In figures 8b-c, for FeAl-2nm/Al-2nm and FeAl-2nm/Al-4nm simulations, both the FeAl and Al layers have been stretched into two parts when the structures are subjected to an applied strain of 15%. However, in figures 8d-e, for the FeAl-5nm/Al-5nm and the FeAl-5nm/Al-10nm simulations at the same strain, the structures are still a whole piece although there are obvious voids formation at the interface and inside the B2 layers. Thus, the deformation response under tensile loading is sensitive to the layer thickness. Void nucleation and coalescence with the increasing strain ultimately led to composites failure. Comparison of figure 8d with 8e also suggests that increasing the layer thickness of the Al layers helps to retard the void formation. Overall, compared to the compressive loading case above, the plastic deformations in the tensile loading case led to more obvious void and crack formation.

3.3 Comparative study of the Fe/Cu multilayer deformation

Earlier atomistic modeling works on dislocation-interface interactions in fcc-bcc semi-coherent interfaces such as Cu/Nb multilayers have shown that the interface barrier to slip transmission depends on the extent of core spreading of dislocations as they enter the interface plane, and this depends on the shear resistance of the interface [8-10,28]. A low shear resistance at the interface (more shearable interface) usually results in the dislocation core spreading at the interface, and as a result, a stronger barrier to the slip transmission [10,28]. Earlier works have shown that relatively low shear strength of the “weak” interface is associated with the positive heats of mixing between the metallic elements in the bilayer metals [28,50].

In Table 2, the calculated heats of mixing as listed show negative values in the FeAl-Al system and positive values in the Fe-Cu system. The heats of mixing (or dilute heats of mixing) describe the energy gain/penalty for placing an atom of one element in the matrix of the other element. When the heat of mixing is positive, a “weak” interface is formed. However, when the heat of mixing is negative, there is enhanced bonding between the two constitutive layers at the interface, thus a “strong” interface is formed. The result of the heats of mixing calculations suggest that the FeAl/Al interface represents a “strong” interface, the Fe/Cu interface maybe considered to

represent a “weak” interface [61]. Thus, it is interesting to have a comparative study of the plastic deformation in the Fe/Cu multilayers.

For the Fe/Cu multilayer deformation study, Fe-5nm/Cu-5nm nanolayered composites with KS orientation relationship was created and MD simulations were carried out under the same loading conditions as in the FeAl/Al simulations, with tensile loading direction along the x direction ($[11\bar{2}]_{\text{Cu}}/[1\bar{1}2]_{\text{Fe}}$). The 5 nm layer thickness sample was chosen in this comparative study (and later on, the detailed examination of void formation processes) was based on consideration of clearer pictures in the deformations in the larger sample size (compared to 2 nm cases, for example). Comparing the stress strain curves of the Fe/Cu and the FeAl/Al nanolaminates in figure 9a, the Fe/Cu multilayers have a higher peak stress and no stress reduction during the whole plastic deformation which is quite different than that of the FeAl/Al multilayers. In figures 9b-c, fracture is observed in the FeAl/Al multilayers while a more homogenous deformation occurs in the Fe/Cu multilayers at the same strain of 25%.

The effect of interfaces on void formation was further studied by comparing dislocation traces (defined by the gliding traces of dislocations left by their movements) within the two interfaces. Figure 10 shows the dislocation traces in the two nanolayered composites. In figure 10a, in the FeAl/Al case, most of dislocations propagate along the interfacial dislocation pattern. Some of the dislocations also interact with the ones in the adjacent parallel interfacial dislocation lines. Thus, short dislocation moving distances are observed in the Al phase. Figure 10b shows that dislocation segments nucleated from the same interface and expanded into the FeAl phase at $\varepsilon_{xx} = 7.056\%$. Atoms are colored according to their z coordinates (heights away from the interface). It reveals that there were only a few dislocation segments in the FeAl phase when void nucleation occurred and elongated in the direction parallel to the interfacial dislocation lines. Note that at strain $\varepsilon_{xx} = 7.056\%$, the void nucleates (with void locations represented by the yellow shapes) at the interface near the interface misfit dislocation lines, as seen in figure 10c. Void nucleation appears in the area of dislocations from the FeAl phase interacting with the interface. The site of void nucleation is not randomly distributed inside the structure and the majority of voids are found to be apart from each other. The elongation of voids coalescence is found to be predominantly along the direction perpendicular to the x axis or the loading direction.

Figures 10d-e show the dislocation traces in the Fe/Cu case at strain $\varepsilon_{xx} = 8.46\%$. In contrast to the FeAl/Al case, the dislocation density in the Fe/Cu multilayers is much higher and the moving distance of dislocation lines is longer (figure 10d) which is consistent with the prior study [62]. At early plastic strains, the activated dislocation slip system in the Cu layer is primarily $1/6[1\bar{1}\bar{2}](\bar{1}1\bar{1})$ and the Schmid factor is 0.1571, which is the same as in the FeAl/Al case. Figure 10e shows that more slip systems are activated in the Fe phase of Fe/Cu than that in the FeAl phase of the FeAl/Al multilayers. There is no void nucleation during the entire plastic deformations in the Fe/Cu simulations. Note that most dislocation traces in the FeAl expanded along the direction normal to the loading direction, which may cause the local shear strain accumulation along that direction. However, dislocation traces in the Fe phase of the Fe/Cu multilayers are relative uniformly distributed, which uniformly accommodates the plastic deformations seen in figure 9c.

The comparative study in the MD simulations reveal that the Fe/Cu multilayers have much improved ductile plastic response compared to FeAl/Al multilayers. This is attributed to much higher dislocation density, more slip systems activated, and relative uniformly distributed dislocation traces in the Fe phase of the Fe/Cu multilayers. The conclusion from this study is in good agreement with the what was drawn from our recent MD simulation study of dislocation impingement and slip transfer at the Fe/Al and Fe/Cu interfaces [61]. In that study, it was shown that for the “weak” Fe/Cu interface, a lot more delocalization occurs at the interface, causing the rather homogeneously spread of plasticity across the material system, even in heavily co-deformed nanoscale multilayers.

3.4 Void formation mechanism in the FeAl/Al nanolaminates

To investigate the void nucleation process, we compared the atomic configurations around the void nucleation region (figure 10c) during deformation responses of FeAl/Al nanolaminates under tensile loading condition. The results are shown in figure 11 and figure 12. Several characterizations have been utilized, including local von Mises shear strain distribution (figure 11 (a)-(d)), the dislocation activities (figure 12 (a1)-(d1)), and the corresponding interface disregistry analysis (figure 12 (a2)-(d2)).

Figure 11 shows the atomic configuration evolution of local shear strain before and after the void nucleation. In figure 11a, dislocation activities have been observed around the void

nucleation area in the Al before the occurrence of void formation. A dislocation with Burgers vector of $1/2[1\bar{1}1]$ nucleated in the FeAl layer and propagated into the interface, as shown in figures 11b and 11c. Then void formation appeared at the interface, in the region where two dislocations interact, as shown in figure 11d.

Further study of the dislocation evolution before and after the void nucleation is carried out. In figure 12 (a1)-(d1), before the void nucleation at strain $\varepsilon_{xx} = 6.99030\%$, in the Al phase, dislocations propagated to and interacted with the interface, while in the FeAl phase, a dislocation denoted by “*i*” has not reached to the interface yet, which is consistent with the local shear strain distribution picture (figure 11a). In figure 12 (a2)-(d2), the disregistry vector is also calculated to characterize the interface defects. The vertical axial is along the *y* direction and the horizontal axis is along the *x* direction. In figure 12 (a2), the disregistry vector is seen to be uniformly distributed except along the interfacial misfit dislocation lines (as analyzed in Section 3.1). As the applied tensile strain increases, the $1/2\langle 111 \rangle$ dislocation in the FeAl layers propagates down to the interface and decomposes into two dislocations. Furthermore, the two decomposed dislocations slip away along the direction normal to the loading direction before another dislocation (denoted by “*ii*”) coming down to the interface as shown in figure 12 (b1). Note that the void nucleation commences after the dislocation “*i*” interacts with the interface, which is associated with strain accumulation there and the corresponding non-uniform interface disregistry vectors at the void region (see figure 12 (a2)-(d2)). The plot of interfacial disregistry vectors also indicates that the void nucleation location and void coalescence process (marked with the dotted purple ellipse) at the interface.

These results suggest that void nucleation is highly related to dislocation activities and the interface structure. Results of dislocation activities leading to the void nucleation appear to agree with the idea proposed in prior study [63] that the void nucleation follow dislocation creation process, while in our cases the dislocation interaction occurred on the interfaces. The examined MD simulations with layer thickness of 5 nm is a representative picture of void nucleation in FeAl/Al multilayers. In addition, while the concept of correlation between void nucleation and dislocation activity is well known in literature, the detailed dynamic process depicting the actual kinetic process in the multilayer deformation response is valuable, contributing to the understanding of the detailed mechanisms in the strain localization induced void nucleation in the intermetallic multilayers. To the author’s knowledge, this is first time that the monitoring of

dislocation activities that contribute to the formation of void nucleation at the intermetallic multilayers is reported.

In order to investigate the effect of void nucleation and growth on dislocation activities during plastic deformation, the percentage of highly shear-strained atoms during deformation responses is analyzed for both the FeAl/Al and the Fe/Cu cases during the tensile load condition. Figure 13 shows the percentage of highly shear-strained atoms with shear strains larger than 0.2 as a function of the applied tensile strain¹. The percentage of highly shear-strained atoms would indicate the magnitude of dislocation traces occurring in the two bulk phases of the multilayer structure. Figure 13 suggests that most of the dislocation traces happened in the Al layers and only a few dislocation activities occurred in the FeAl layers. We can deduce that the plastic deformations of the Fe/Cu and FeAl/Al multilayers are compensated primarily by dislocation activities. At larger applied strains, for the FeAl/Al nanocomposite, fewer dislocation traces happened due to the suppression by void growth and coalescence (in comparison, the percentage of highly shear-strained atoms in the Fe/Cu case increases with the increment of applied strains during the whole plastic deformation process). Furthermore, the percentage of highly shear-strained atoms in the FeAl phase has a relatively smaller increment after about strain at 12%. In the meantime, we can approximate the fraction of void volume using the construction of surface mesh in OVITO software. Green line in figure 13 shows the fraction of void volume as a function of the applied strain in the FeAl/Al multilayers. It suggests that the fraction of void volume increases with the applied tensile strains, thus offering a strong justification for the observed difference in the percentage of highly strained atoms as due to the void formation in the FeAl/Al multilayers. The deformation is primarily accommodated by fracture, rather than the plastic flow, at large strains.

4. Conclusions

The deformation response of the B2-FeAl/Al intermetallic composites, in KS orientation relationship, has been studied using MD simulations. Both loading conditions have been applied during the MD simulations, including uniaxial compressive loading normal to the interface and

¹ The value of 0.2 (or 20%) of the applied tensile strains was chosen based on the observation of the values of von Mises shear strain of the dislocation atoms are larger than ~ 0.2 .

tensile loading parallel to the interface. A comparative study of the deformation response of the Fe/Cu nanolaminates in KS orientation relationship has also been carried out. The atomistic modeling study on the nanolayered composites comprised of intermetallic interfaces and their deformation responses studied underpinned the mechanical response of “strong” intermetallic interface material systems. The major results are summarized as follows:

- (1) From F-B equation analysis, two sets of dislocations as the interface misfit dislocation content at the interface were identified, with one set of dislocation with strong core-overlap and mainly of edge type character while the other set of dislocations in distant distance away from each other and more of screw type character.
- (2) The nucleation sites of dislocations are from the Al side of the interface, with activated slip systems having a positive large Schmid factor and correlates with the misfit dislocation lines. Of the nucleated dislocations, some dislocations propagate in the form of two Shockley partials $1/6\langle 112 \rangle$ and stair-rod dislocation $1/6\langle 110 \rangle$ and expand into the Al layers.
- (3) The compressive study shows that the higher B2-FeAl fraction leads to the strengthening of the nanocomposites. The dislocations of Shockley partials in fcc and dislocations of $1/2\langle 111 \rangle$ in B2-FeAl structures are the dislocations that primarily accommodate the plastic deformation.
- (4) Compared to the compressive loading case above, the plastic deformations in the tensile loading case in FeAl/Al nanolaminates led to more obvious void and crack formation. Void nucleation process was investigated and interface structure with dislocation activities are suggested to play a significant role to trigger the strain delocalization, leading to initial void nucleation at the interfaces.
- (5) The deformation behavior in the “weak” interface Fe/Cu nanolaminates behaves substantially different than that of the “strong” interface FeAl/Al samples. There is no void nucleation during the entire plastic deformations in the Fe/Cu simulations. This is attributed to much higher dislocation density, more slip systems activated, and relative uniformly distributed dislocation traces in the Fe phase of the Fe/Cu multilayers.

Acknowledgements

S.D. and C.Z. acknowledge the financial support by NSF CAREER Award (CMMI- 2015598). This work was also partially supported by the Los Alamos National Laboratory (LANL) Directed Research and Development Program 20200182DR. LANL is operated by Triad National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under Contract No. 89233218CNA000001.

Declarations

Conflict of interest: The authors declare no conflicts of interest.

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