

Research Article

Microstructure evolution and deformation mechanism of amorphous/crystalline high-entropy-alloy composites

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ABSTRACT

High-entropy amorphous alloys present high hardness, but low tensile ductility. Here, deformation behavior of the amorphous/crystalline FeCoCrNi high-entropy alloy (HEA) composite prepared by the previous experiment is investigated using atomic simulations. The result shows the partial dislocations in the crystal HEA layer, and the formation of shear bands in the amorphous HEA layer occurs after yielding. The strength of the amorphous/crystalline HEA composite reduces with increasing the thickness of the amorphous layer, agreeing with the previous experiments. The coupled interaction between the crystal plasticity and amorphous plasticity in amorphous/crystalline HEA composites results in a more homogeneous redistribution of plastic deformation to cause interface hardening, due to the complex stress field in the amorphous layer. The current findings provide the insight into the deformation behavior of the amorphous/crystalline HEA composite at the nanoscale, which are useful for optimizing the structure of the HEA composite with high strength and good plasticity.

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1. Introduction

High-entropy alloys (HEAs), consisting of five or more elements with equiatomic or near-equiatomic concentration, are widely investigated due to their exceptional mechanical properties, e.g., high strength and hardness [1–4]. In general, the experimental results demonstrate that HEAs tend to form simple solid-solution structures or multi-phase structures due to their high mixing entropy [5–7]. Recently, the high-entropy bulk metallic glasses have been developed by the rapid cooling method [8–12]. The HE-BMGs, the combination of HEAs and bulk metallic glasses (BMGs), which have both strong topological and chemical disorder, show some unique or remarkably improved properties, compared with the normal BMGs or HEAs [13,14].

To improve the mechanical properties in BMG composites, the amorphous–crystalline multilayered structures are fabricated by the magnetron sputter deposition of alternating layers of various metals [1–17]. By a controlled growth of crystalline and

amorphous phases, the deformation behaviors are systematically studied [18–20]. For example, in the amorphous/nanocrystalline (e.g., CuZr/Cu) composite, a multilayer structure can suppress the formation of shear bands and enable plastic co-deformation of the two phases [21–24]. The effects of layer thickness and sample size on the deformation behavior of crystalline/amorphous Cu/CuZr composites under tension loading are investigated using a molecular dynamics (MD) simulation method. The peak stress reaches a plateau when the crystal layer thickness is larger than 5 nm [21]. The effect of grain-boundary characteristics on the atomistic mechanisms of yielding and plastic deformation behavior is constructed. It demonstrates a transition of the deformation mode from the localized to homogeneous-like deformation by tailoring the relative volume fraction of the Cu layers [22]. Using a systematic experiment and MD simulation, a transition of deformation modes from shear banding to co-deformation subject to nanoinindentation was revealed by a systematic experimental study of the amorphous/crystalline composite [23,24]. In those investigations, the crystalline and amorphous layers usually remained of equal thickness, and thus, the transition of deformation behaviors may emerge from the length-scale effect of both amorphous and crystalline phases [25,26]. Recently, the amorphous/crystalline HEA FeCrCoNi has been successfully prepared by the high-pressure tor-

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sion (see Fig. 1(a)) [8]. More recently, the HEA coated with the amorphous films represents the high yielding strength and ultimate tensile strength attributed to the limitation of the dislocation nucleation and mobility by the back stress and repulsive image stress at the interface [27–29]. The structural hierarchy of AlCoCr-CuFeNi HEA can be obtained by controlling cooling rates, and the mechanical behavior of HEA composite is optimized to maximize high strength [30]. However, up to now, little work has been conducted concerning the influence of the amorphous layer thickness on the mechanical properties in the amorphous/crystalline HEA composite.

In the present work, the deformation behavior in the amorphous/crystalline HEA FeCrCoNi composite of varying amorphous layer thicknesses is investigated using the MD simulation method. The structural/interfacial evolution, shear strain, and stress have been studied to reveal the thickness effect of the amorphous HEA layer on the mechanical properties.

2. Simulation model and method

Fig. 1(b) and (c) shows the tension simulations of amorphous/crystalline HEA FeCrCoNi structures. This model includes the amorphous HEA and crystalline HEA. The dimension of the sample is $15.5 \text{ nm} \times 15.2 \text{ nm} \times 16.1 \text{ nm}$. To investigate the effect of size on the tensile deformation in the amorphous/crystalline HEA composite, the various amorphous HEA layer thicknesses can range from 0 to 15.5 nm. The amorphous/crystalline HEA FeCrCoNi is randomly distributed with Fe, Co, Cr, and Ni atoms. To obtain the amorphous HEA model, it is melted at 2500 K in the isobaric–isothermal ensemble (NPT) first, then quenched from 2500 K to 300 K at a cooling rate of 10 K/ps [21–24,30]. According to the experiment [8], the crystallographic orientation of the crystalline HEA layer is set as [011] along the x -axis, [1–11] along the y -axis, and [21,1] along the z -axis. Periodic boundary conditions are applied along x , y , and z directions. The embedded atom method (EAM) potential is widely used to study the solidification, microstructure evolution, and plastic deformation driven by tension [30–34]. Using the current EAM potential, some works have studied the microstructure evolution, mechanical properties, and strengthening mechanism in single crystal HEA [34], dual-phase HEA [6], nanocrystalline HEA [35] and amorphous HEA [36,37].

The initial temperature of MD simulations in the amorphous/crystalline HEA FeCrCoNi composite is 300 K. Before the tension, the sample is first subjected to the energy minimization using the conjugate gradient method [6,34–36], and then all relaxed to obtain an equilibrium state. The constant strain rate of $1 \times 10^8 \text{ s}^{-1}$ is applied along the x -direction [34–36]. A time step is 1 fs in all MD simulations, using the large-scale atomic/molecular massively-parallel simulator (LAMMPS) [38]. The microstructural evolution is

presented via the Ovito software [39]. The common neighbor analysis (CNA) is used to identify the microstructure after deformation, where red atoms represent the stacking fault, green atoms mean the face-centered cubic (FCC) structure, and the white atoms are the dislocation core and interface structure as well as amorphous structure.

3. Results

According to the previous work [21–23], the layer thickness of a crystal structure plays a key role in the mechanical properties and deformation mechanisms in crystalline/amorphous composites. The stress-strain curves of the amorphous/crystalline HEA FeCrCoNi composite with different amorphous layer thicknesses are presented in Fig. 2(a), where the thicknesses of the amorphous HEA layer are 0 nm, 3 nm, 6 nm, 9 nm, 12 nm, and 15.5 nm. The corresponding volume fractions between the amorphous HEA layer and composite are 0%, 19.4%, 38.7%, 58.1%, 77.4%, and 100%. Apart from the amorphous HEA, the deformation of the amorphous/crystalline HEA with varying thicknesses suffers with the elastic stage, yielding stage, softening stage, and hardening stage (Fig. 2(a)). In the amorphous/crystalline HEA composite, the crystalline HEA has the high strength, followed by the amorphous/crystal structure, and finally amorphous structure. This result agrees with the report in crystalline Cu/amorphous Cu50Zr50 composites, where the strength of the crystalline Cu is higher than that of the amorphous Cu50Zr50 [21]. Moreover, with the increasing thickness of the HE-BMG layer, the strength of the HE-BMG/crystalline sample reduces, in good agreement with the experiment results in the amorphous Cu45Zr55/crystalline Cu [23]. As can be found, the single crystal HEA samples possess the high yielding strength, compared to their amorphous counterparts. The similar results are observed in the stress–strain curves of amorphous/crystalline Au nanowires, Mg alloys, CuAg alloys, and CuZr alloys [40–43]. This trend is attributed to the strong size effect in the single crystal sample [44]. However, the traditional bulk alloys present coarse-grained/fine-grained structures, which have a low strength compared to their amorphous counterparts owing to the nucleation of voids or cracks from grain boundary, and grain boundary sliding at a low critical threshold stress [45–47].

Using the mixed principle, the flow stress of multilayers can be estimated by $\sigma = \sigma_a t_a / (t_a + t_c) + \sigma_c t_c / (t_a + t_c)$ [23], where σ_a and σ_c represent the flow stresses of the amorphous and crystalline HEA, respectively. t_a and t_c represent the thicknesses of the amorphous and crystalline HEA layers, respectively. Here, the flow stress decreases with the increasing thickness of the amorphous HEA, consistent with the result of Fig. 2(a). It can be noted that the stress significantly drops in the sample with the small thickness of the amorphous HEA layer after yielding (Fig. 2(a)). On the other

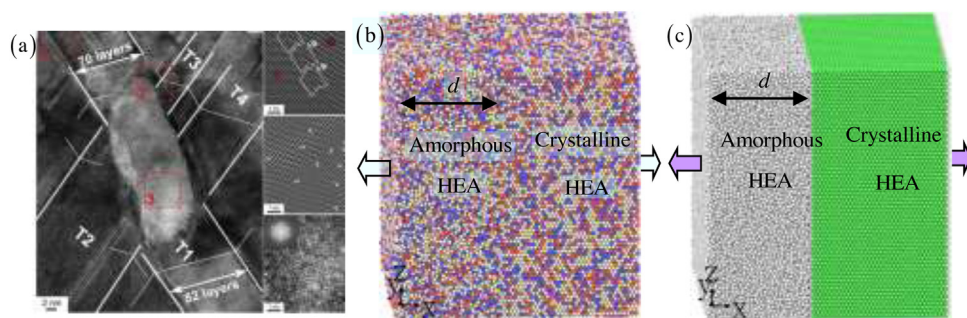


Fig. 1. (a) The amorphous/crystalline HEA FeCrCoNi composite prepared by high-pressure torsion from the experiment [8] and (b, c) the tension model of the amorphous/crystalline HEA structures (● Fe, ● Co, ● Cr, and ● Ni). The atoms are colored by the atom types (b). The atoms are represented by different colors based on the structure types (c).

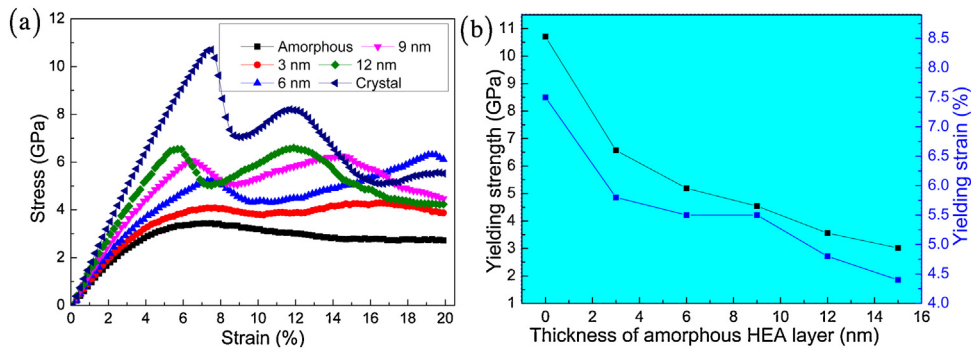


Fig. 2. Stress vs. strain in the amorphous, crystal, and amorphous/crystal HEA at different thicknesses of the amorphous HEA layer (a) and yielding strength and strain at different thicknesses of the amorphous HEA layers (b).

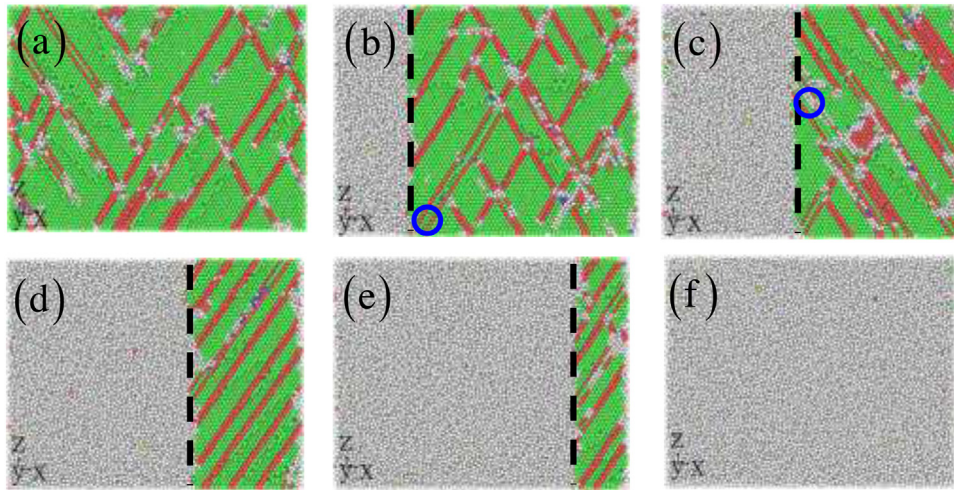


Fig. 3. The structural evolution at the strain of 20% and different materials: the crystalline HEA (a), the amorphous HEA layer with 3 nm (b), the amorphous HEA layer with 6 nm (c), the amorphous HEA layer with 9 nm (d), the amorphous HEA layer with 12 nm (e), and the amorphous HEA (f) at a strain of 20%. Dotted lines represent interfaces.

hand, the yielding strain increases with the decreasing thickness of the amorphous HEA layer (Fig. 2(b)), indicating the softening in advance. Hence, the thickness of the amorphous HEA layer plays a critical role in the overall mechanical response under tensile deformation.

To reveal the underlying deformation mechanism of the amorphous/crystal HEA composite considering the effect of the amorphous HEA layer, the atomic structures of amorphous/crystal HEA composites at the tensile strain of 20% are presented in Fig. 3. The nucleation of the Shockley partial dislocation could occur at the crystalline–amorphous interface, and then Shockley partial dislocations are absorbed at the opposite interface in Fig. 3(b–g). The corresponding dislocation densities are $7.28 \times 10^{17} \text{ m}^{-2}$, $6.68 \times 10^{17} \text{ m}^{-2}$, $5.18 \times 10^{17} \text{ m}^{-2}$, $9.62 \times 10^{17} \text{ m}^{-2}$, $1.35 \times 10^{17} \text{ m}^{-2}$, and $4.32 \times 10^{17} \text{ m}^{-2}$ in Fig. 3, in addition to the pure amorphous HEA. With the increasing thickness of the amorphous HEA layer, the dislocation density dynamically fluctuates, exhibiting different degrees of plastic deformation in the crystalline layer. It is confirmed that the deformation behavior of the crystal layer has a good correlation to the dislocation density [48,49], and depends on the thickness of the amorphous HEA layer. By comparing Figs 2 and 3, the high strength mainly comes from the contribution of the crystalline HEA layer through the dislocation hardening mechanism, and the nucleation and slip of dislocations in the crystalline HEA layer further activate plasticity in the amorphous HEA layer [40–43]. Especially, the deformation twins occur at the interface (Figs 3 and 4), which strongly affects the mechanical properties of the amorphous/crystal HEA composite [8,30]. More-

over, the dislocation nucleation leads to the non-smooth interface structure (Fig. 5). Here, for different thicknesses of the amorphous HEA layers, the interface morphology is presented in Fig. 5(a–f), and the atomic displacement is shown in Fig. 5(g–l), to reveal the fluctuation of the interface morphology on the deformation behavior. The red atom means the high atomic displacement, and the blue atom indicates the low atomic displacement. As a result, the strip texture generates in the non-smooth interface, which provides nucleation sites for the shear-band embryo (Fig. 6).

4. Discussion

In order to obtain the deep understanding of the influence of microstructures on the deformation behavior [21–23], the atomic shear strain of the amorphous/crystal HEA composites is calculated after the tensile deformation. Fig. 6(a–d) displays the distribution of the atomic shear strain after the deformation at the total strain of 20%. The shear strain is computed by determining the deformation gradient tensor from the initial and current atomic positions. The red atom means a high shear strain, and the blue atom indicates a low shear strain. The obvious main shear bands are observed in the crystalline layer, and a large number of tiny shear bands occur in the amorphous HEA. Moreover, the high shear strain in the amorphous HEA layer is concentrated in the interface region. The shear band does not penetrate the interface from the crystalline to amorphous HEAs, which is different with the previous report about the shear band across the crystal and amorphous structure in the multilayer amorphous Cu₅₀Zr₅₀/Cu nanolaminated compos-

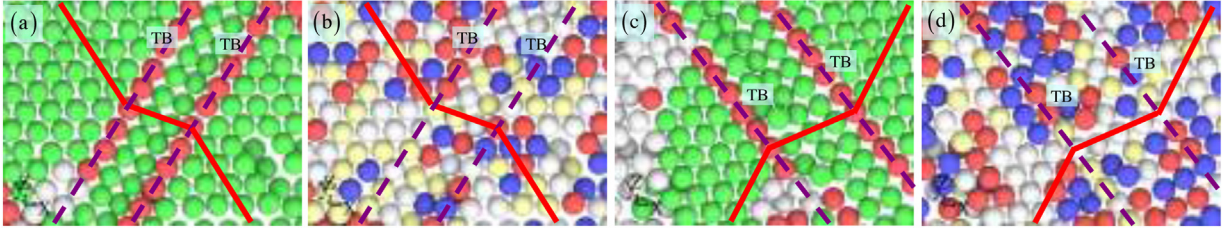


Fig. 4. The deformation twins at the strain of 20 % and different amorphous HEA layers: (a, b) 3 nm; (c, d) 6 nm. This region is marked by the blue circles in Fig. 3. TB represents the deformation twin boundary.

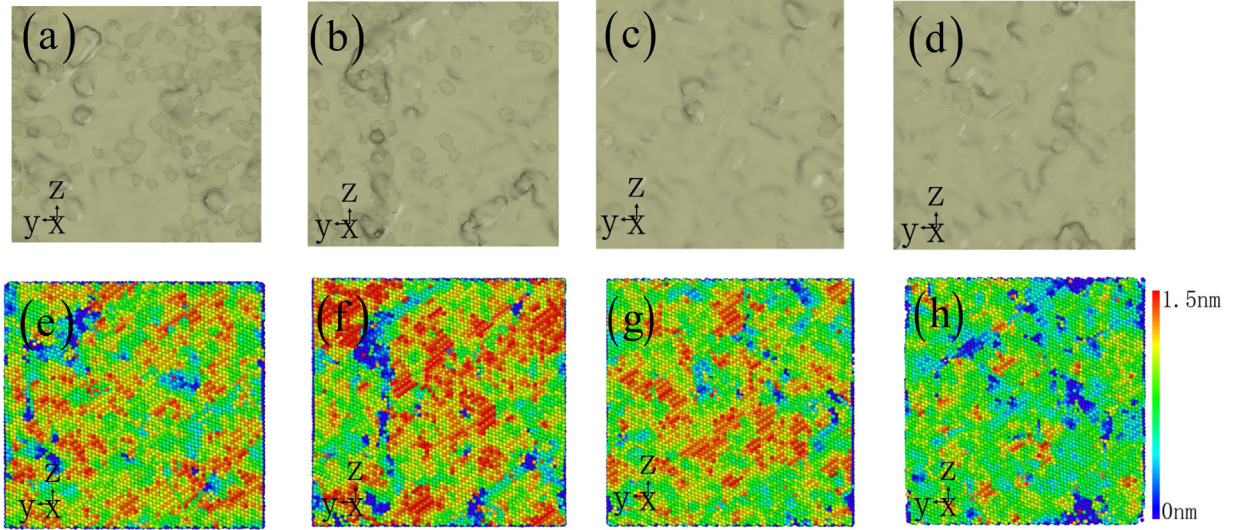


Fig. 5. The interface morphology in the strain of 20% and different amorphous HEA layers: (a, e) amorphous HEA layer with 3 nm; (b, f) amorphous HEA layer with 6 nm; (c, g) amorphous HEA layer with 9 nm; (d, h) amorphous HEA layer with 12 nm. (a-d) represent the surface morphology of the interface, and (e-h) represent the atom displacement from the interface.

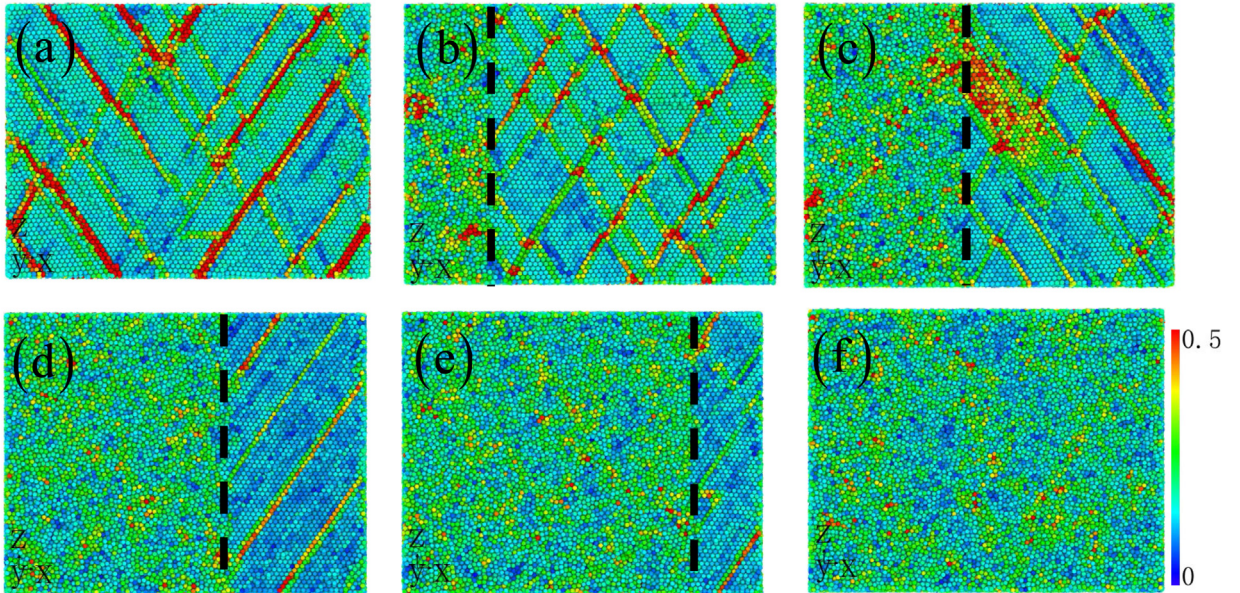


Fig. 6. The shear strain distribution at the strain of 20% and different materials: the crystalline HEA (a), amorphous HEA layer with 3 nm (b), amorphous HEA layer with 6 nm (c), amorphous HEA layer with 9 nm (d), amorphous HEA layer with 12 nm (e), and amorphous HEA (f). Dotted lines represent interfaces.

ites [22]. The dislocation nucleation induces the formation of shear bands, which could be proved in the high strain located at the contact interface between the dislocation and amorphous HEA (Fig. 6). Hence, the slip mechanism is found in the amorphous/crystal

HEA composites, to enhance the plastic ability of the amorphous HEA.

The local stress concentration plays a decisive role in the deformation behavior, leading to controlled mechanical properties. Here,

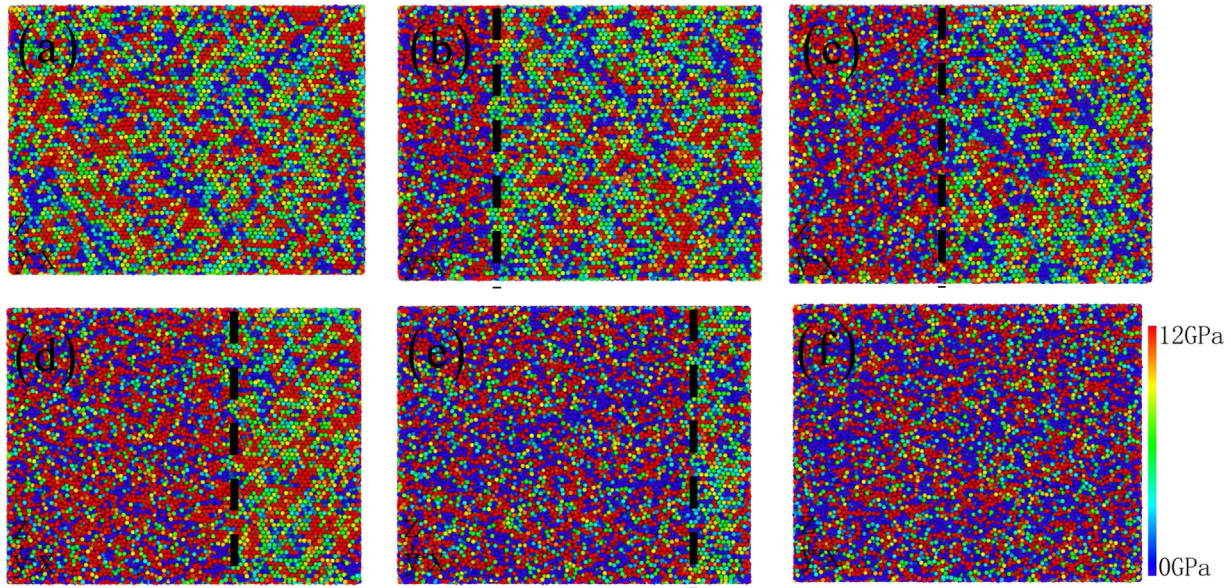


Fig. 7. The stress distribution at the strain of 20% and different materials: the crystalline HEA (a), amorphous HEA layer with 3 nm (b), amorphous HEA layer with 6 nm (c), amorphous HEA layer with 9 nm (d), amorphous HEA layer with 12 nm (e), and amorphous HEA (f). Dotted line represents the interface.

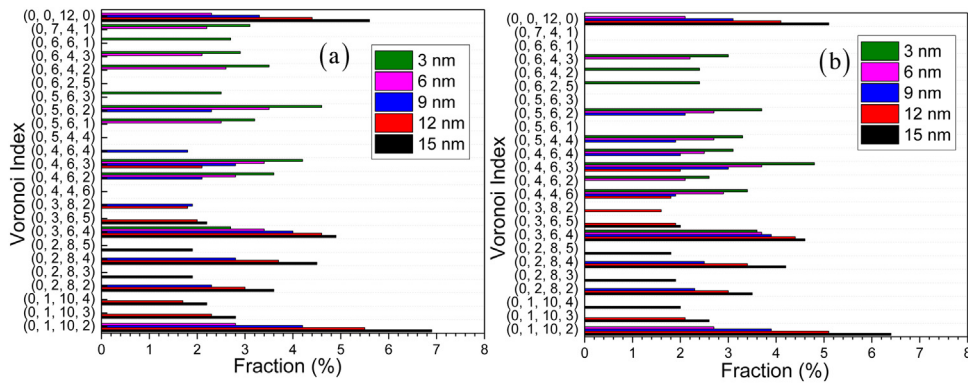


Fig. 8. Distribution and proportion of major VPs before deformation (a) and after deformation (b) at different amorphous HEA layers.

the distribution of the stress along the x direction is shown in Fig. 7. The red atom means the high tensile stress, the blue atom indicates the high compressive stress, and the green atom represents the low or free stress. Compared to the crystalline HEA layer, the amorphous HEA layer presents a more complex stress distribution, where the local high tensile and compressive stresses alternately appear in the loading plane. Meanwhile, the crystalline HEA shows the relatively stable and low peak in the stress distribution. This trend is due to that the amorphous HEA has the random distribution of different elements with various atomic radii [1–6]. The shear bands are very difficult to pass through the interface, due to the complex stress fields. Furthermore, the local stress gradient drives the deformation behavior, to control the mechanical properties, especially the softening effect. Hence, the fluctuation of the stress from the tensile to compressive stresses in the range of several Ångström scales along the interface, controls the slip of dislocations in the crystalline layer and the formation of shear bands in the amorphous HEA layer. This trend leads to a more homogeneous redistribution of plastic deformation (Figs 3–7). A comparison of Figs 6 and 7 shows the universal phenomenon of the local yield in the amorphous HEA layer due to the different atomic bond strengths. It can govern the interface properties, which control both the thickness-dependent global yield strength and strain hardening of the amorphous/crystal HEA composite.

To characterize the local structure of the deformed HEA, the Voronoi polyhedron method (VPM) is employed to identify the structure according to the previous study [50–52]. The VP can be indexed as $\langle n_3, n_4, n_5, n_6, \dots, n_i \rangle$, where n_i represents the number of i -edge faces on the VP [50–52]. The majority of VPs can be denoted by a 4-integer index $\langle n_3, n_4, n_5, n_6 \rangle$ [50]. In addition, the vertex is ignored if the number of atoms in the VP is less than 1% of the total. Fig. 8 shows the distribution and proportion of VPs in deformed HEA. When the amorphous HEA layer is larger than 9 nm, the top three VPs are $\langle 0, 1, 10, 2 \rangle$, $\langle 0, 3, 6, 4 \rangle$ and $\langle 0, 0, 12, 0 \rangle$ before the deformation (Fig. 8(a)), and after the deformation (Fig. 8(b)). When the amorphous HEA layer is lower than 6 nm, $\langle 0, 4, 6, 3 \rangle$ and $\langle 0, 5, 6, 2 \rangle$ in the top two VPs take place. With increasing amorphous HEA layer, the VPs of $\langle 0, 3, 8, 2 \rangle$, $\langle 0, 4, 4, 6 \rangle$, $\langle 0, 4, 6, 2 \rangle$, $\langle 0, 4, 6, 3 \rangle$, $\langle 0, 4, 6, 4 \rangle$, $\langle 0, 5, 4, 4 \rangle$, $\langle 0, 5, 6, 1 \rangle$, $\langle 0, 5, 6, 2 \rangle$, $\langle 0, 5, 6, 3 \rangle$, $\langle 0, 6, 2, 5 \rangle$, $\langle 0, 6, 4, 2 \rangle$, $\langle 0, 6, 4, 3 \rangle$, $\langle 0, 6, 6, 1 \rangle$, $\langle 0, 7, 4, 1 \rangle$ increase, and the VPs of $\langle 0, 1, 10, 2 \rangle$, $\langle 0, 1, 10, 3 \rangle$, $\langle 0, 1, 10, 4 \rangle$, $\langle 0, 2, 8, 2 \rangle$, $\langle 0, 2, 8, 3 \rangle$, $\langle 0, 2, 8, 4 \rangle$, $\langle 0, 2, 8, 5 \rangle$, $\langle 0, 3, 6, 4 \rangle$, $\langle 0, 3, 6, 5 \rangle$ decrease. When the amorphous HEA layer decreases to 3 nm, new VPs of $\langle 0, 6, 6, 1 \rangle$ and $\langle 0, 7, 4, 1 \rangle$ occur. Compared to VPs in the deformed HEA before the deformation, a similar distribution and proportion of VPs can be observed in the deformed HEA after the deformation (Fig. 8(b)), in addition to VPs of $\langle 0, 4, 4, 6 \rangle$, $\langle 0, 5, 4, 4 \rangle$, $\langle 0, 4, 4, 6 \rangle$, and $\langle 0, 6, 2, 5 \rangle$. Moreover, these VPs only exit in a

deformed HEA, and the VPs of <0, 1, 10, 4>, <0, 3, 8, 2>, <0, 5, 6, 1>, <0, 5, 6, 3>, and <0, 7, 4, 1> only exit in an undeformed HEA. Thus, the VP evolution depends on the thickness of the amorphous HEA layer, and then regulates the mechanical properties.

5. Conclusion

In the current work, the deformation behaviors and mechanical properties in amorphous/crystal HEA composites are investigated by means of MD simulations. The effects of the amorphous HEA layer thickness on the tensile deformation behavior are systematically studied. The dislocation nucleation in the crystal HEA layers and the formation of multiple embryonic shear bands in the amorphous HEA layers take place after plastic deformation. The strength of amorphous/crystal HEA composites reduces with increasing the thickness of the amorphous layer. This trend agrees with not only the previous experimental results in the amorphous Cu₄₅Zr₅₅/crystalline Cu, but also the mixed principle of a simple composite average. Furthermore, the softening stress and the yielding strain increase, as the thickness of the amorphous HEA layer decreases. The origin of the high plasticity is attributed to the enhanced redistribution of plasticity, by the coupled interaction between the crystal plasticity, and the glassy plasticity at the nanoscale. This deformation mechanism results in the high yielding strength in the nanolaminated composites. Moreover, tailoring the thickness of the amorphous layers would be an effective way, for tuning the plasticity of nanolaminated composites. The results provide the fundamental understanding the underlying atomistic mechanisms of yielding and tunable plasticity, which guide the design of the amorphous HEA with the high strength and good plasticity.

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