Atomistic study of plastic deformation in Mg–Al alloys

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ABSTRACT

An atomistic study has been carried out to understand plastic deformation in Mg–Al alloys. We investigate the possible plastic deformation mechanisms of intermetallic β -Mg₁₇Al₁₂ which is a key precipitate phase in Mg–Al alloys. Based on the analysis of the generalized stacking fault energy, we predict the preferential slip systems in this phase and speculate that partial dislocations and complex stacking faults are responsible for its plastic deformation. Using Rice's criterion on ductile-to-brittle transitions, we confirm the intrinsic brittleness of the intermetallic phase. We also simulate the interaction between the basal edge dislocation and dissolved Al particles. We have determined the binding energy between the dislocation and the particles and examined the energetic dependence on the particle size, particle concentration and dislocation–particle distance. The strengthening effect due to the Al solutes is characterized by two quantities – the Peierls stress and the solid solution strengthening factor. The former reflects the changes in dislocation core structure while the latter results primarily from the elastic dislocation–particle interaction. Both quantities are examined and their dependence on particle size and concentration is elucidated. The dislocation core structure and the long-range elastic interaction between the dislocation and the Al particles are also examined.

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1. Introduction

The applications of lightweight structural materials in automobile and aerospace industries represent an effective measure to conserve energy and reduce carbon dioxide emissions. Magnesium alloys, known for their lightweight, highly specific stiffness and excellent casting capability, are prime candidates for such applications [1]. Aluminum constitutes the main alloying element to improve the mechanical properties of Mg alloys, providing enhanced die castability, corrosion resistance, and a good combination of mechanical properties at room temperature [2–4]. One prominent example is Mg–Al–Zn alloy (AZ91) which is one of the most popular commercial Mg alloys. In Mg–Al alloys, Al can be dissolved into Mg matrix, resulting in solid solution strengthening in either the as-cast state or at low Al contents. Al can also precipitate into a stable intermetallic β -phase Mg₁₇Al₁₂ as the Al content increases. The intermetallic β -Mg₁₇Al₁₂ is the dominant precipitate phase in Mg–Al alloys [5,6] and it can greatly influence the mechanical properties of Mg–Al alloys [2,5,7,8].

In this paper, we study the plastic deformation mechanism of the intermetallic Mg₁₇Al₁₂ phase and solid solution strengthening of dissolved Al particles in Mg–Al alloys by atomistic simulations. Both problems are important to the mechanical properties of Mg–Al

alloys notwithstanding they play drastically different roles in the plastic deformation. In the first problem, we focus on the generalized stacking fault energies of Mg₁₇Al₁₂ phase, and explore the possible plastic deformation mechanisms at the atomic scale. Based on Rice's criterion of ductile-to-brittle transitions, we are able to firmly establish the intrinsic brittleness of the intermetallic phase, resolving an apparent controversy between theory and experiment. In the second problem, we determine the interaction between a basal edge dislocation and dissolved Al particles using both atomistic calculations and simple elastic analysis. We elucidate the solid solution strengthening effect due to the Al particles by examining the dislocation core structure and the Peierls stress, as well as the solid solution strengthening factor.

2. Methodology

Generalized stacking fault energy surface (or γ -surface) captures the atomistic interaction across dislocation slip plane and is responsible for dislocation core properties. As a result, the γ -surface has been widely used to provide quantitative analysis of dislocation core structure, particularly in the context of Peierls–Nabarro model [9–11]. Here, we calculate γ -surfaces for Mg₁₇Al₁₂ phase using both first-principles and classical atomistic simulations, which allow us to gain physical insight of plastic deformation mechanism without modeling the dislocations explicitly. In the first-principles calculations, we have used the Vienna *Ab initio* Simulation Package (VASP) [12,13] based on

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the density functional theory (DFT) and plane-wave pseudopotential formalism. The electron–ion interaction is described by the projector augmented wave method [14,15] and the exchange–correlation potential is determined by generalized gradient approximation in Perdew–Burke–Ernzerhof form [16]. Similar to Lu et al.'s [9], three dimensional periodic boundary conditions are employed to the supercell with dimensions of $l \times \sqrt{2}l \times \sqrt{2}l$, consisting of 68 Mg atoms and 48 Al atoms; l is the lattice constant of the body-centered-cubic (b.c.c.) β -Mg₁₇Al₁₂. A $(6 \times 4 \times 4)$ k -point mesh in Monkhorst-Pack scheme is used in sampling the Brillouin zone and the energy cutoff of the plane-wave basis is 320 eV. In the classical simulations of the γ -energy, we have used the Embedded-Atom-Method (EAM) developed by Liu et al. [17] with the periodical boundary conditions applied in three dimensions.

To examine solid solution strengthening effect due to Al solutes in Mg matrix, we have modeled Al (a single Al atom and two Al nanoparticles) interacting with an edge dislocation in the basal plane of Mg by static EAM calculations. Thanks to its highest mobility among dislocations in Mg, the edge dislocation in the basal plane plays a crucial role in the plastic deformation of Mg and Mg alloys. The lattice parameters of the hexagonal-close-packed (h.c.p.) Mg matrix are $a_0 = 3.196 \text{ \AA}$ and $c_0 = 5.187 \text{ \AA}$. The Burgers vector of the basal edge dislocation is $(a_0/3)[1\bar{1}20]$ along X direction; the slip plane normal is $[0001]$ along Y direction, and the dislocation line is along $[1\bar{1}00]$ (Z) direction. The dimensions of the supercell along X , Y and Z directions are $100a_0 \times 60c_0 \times L\sqrt{3}a_0$ where $L=20$ and 100 , corresponding to two different dislocation lengths with 0.48 million and 2.4 millions atoms in total. The periodic boundary condition is applied in Z direction and the open boundary conditions are employed in the other two directions. In the presence of Al atoms, L would also represent the inter-particle distance scaled by $\sqrt{3}a_0$.

The binding energy $E_b(n\text{Al}, \text{disl})$ is defined as the total energy of the dislocation in the presence of a nearby Al particle relative to the total energy of the dislocation with the particle infinitely away. In practice, we calculate the total energy as a function of increasing dislocation–particle distance until the energy converges to less than 0.001 eV. We then set the total energy at the largest dislocation–particle distance as the reference (or zero energy) point, relative to which the binding energies at intermediate distances are determined. If the binding energy $E_b(n\text{Al}, \text{disl})$ is positive (or negative), the Al particle would repel (or attract) the dislocation.

Finally, we have also calculated the Peierls stress for the dislocation by applying shear strains to the supercell. A shear displacement in X direction is introduced to the atoms at the top- and bottom-layer (with the maximum and minimum Y values) of the supercell and remains fixed during the relaxation. Other atoms can relax in all three directions. The Peierls stress is defined as the critical stress under which the dislocation center translates for more than $1b$ from

its initial position. The Peierls stress is then calculated as the sum of the net force in X direction for the atoms on the top-layer divided by the surface area.

3. Results and discussion

3.1. Plastic deformation mechanism and intrinsic brittleness of Mg₁₇Al₁₂ phase

Among Mg–Al binary compounds, Mg₁₇Al₁₂ is the only stable phase at 0 K [18]; Mg₁₇Al₁₂ phase crystallizes in b.c.c. structure consisting of 34 Mg atoms and 24 Al atoms in the unit cell. The calculated lattice constant is 10.42 Å and 10.52 Å from EAM and DFT, respectively, similar to the values obtained by others [19–21]. Despite the importance of Mg₁₇Al₁₂ phase on the mechanical properties of Mg–Al alloys, the basic plastic behavior of Mg₁₇Al₁₂ is not understood.

According to the Peierls–Nabarro model, the dislocation core properties can be determined from the knowledge of γ -surfaces and elastic parameters of the material. However, owing to the complex crystal structure of Mg₁₇Al₁₂, the identification of its preferential slip systems is far from obvious. Hence we first carry out a number of EAM γ -energy calculations to identify the preferential slip systems. Specifically, we focus on five plausible slip systems: $(100)[100]$, $(110)[110]$, $(110)[001]$, $(111)[110]$ and $(111)[1\bar{1}2]$. For each slip system, there are many possible slip planes with unique γ -surfaces. For example, three sets of (010) -type atomic planes are shown in Fig. 1(b) with dashed lines; the interplanar distances between two adjacent atomic planes are labeled as d_1 , d_2 and d_3 . For each set of the two adjacent planes, there is a geometric slip plane at the mid-point between them. The γ -energy curves for each slip system are shown in Fig. 2(a)–(e). Each energy curve is associated with a possible slip plane, identified by an integer number i , so that the interplanar distance is approximately $i\% \times l$, where l is the lattice constant. Three examples of d_1 , d_2 and d_3 are shown in Fig. 2(a). In contrast to simple crystal structures, a larger i value here does not always yield lower γ -energies. Comparing all γ -energy curves, we find that the 110 slip system with the slip plane identified by $i=145$ has the lowest overall γ -energies as shown in Fig. 2(b). The slip plane is indicated in Fig. 1(b) by a solid line with an interplanar distance of 1.5 Å, among the largest interplanar distances in Mg₁₇Al₁₂. The γ -energy curve has a reflection symmetry in $[110]$ direction with a maximum at the center, along with two local minima (maxima). The positions of atoms immediately above and below this slip plane are displayed in Fig. 1(c), with the larger spheres representing Mg atoms above the slip plane and the smaller spheres for Mg atoms below the slip plane. At a fractional displacement of 0.2 indicated by the black arrows, Mg1 atom

Fig. 1. (a) The crystal structure of the intermetallic phase Mg₁₇Al₁₂. The green and red circles represent Mg and Al atoms, respectively. (b) The side view of the crystal structure along $[001]$ direction; the solid line represents the preferential (110) slip plane. The interplanar distances between three pairs of (010) planes are labeled by d_1 , d_2 and d_3 respectively. (c) The atomic positions across the (110) slip plane. The large (small) circles represent Mg atoms above (below) the slip plane; some of the atoms are also displayed in (b). The dashed box indicates the neighboring unit cell. Black and red arrows represent two different slips in $[110]$ direction, corresponding to the two γ -energy maxima in Fig. 2(b). (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

Fig. 2. The γ -energy curves for the five different slip systems. Each curve is labeled by an integer i which quantifies the interplanar distance. The fractional distance is given in terms of the corresponding Burgers vector.

slides to the top of Mg5 atom, and Mg3 atom shifts to the top of Mg7 atom, yielding the local maxima in γ -energy. At a fractional displacement of 0.5 indicated by the red arrows, four pairs of wrong bonds are formed, including Mg1 on top of Mg6, Mg3 on top of Mg8, Mg2 on top of Mg5, and Mg4 on top of Mg7. These on-top positions produce Mg–Mg distances that are too short comparing to the equilibrium value, giving rise to higher stacking fault energies. This is similar to the run-on stacking fault energy observed in Al [9]. The second lowest γ -energy curve belongs to the [001](110) slip system shown in Fig. 2(c) with slightly higher γ -energies than the 110 slip system.

Having identified the preferential slip systems, we perform further DFT calculations to (i) confirm the EAM results and (ii) obtain more accurate γ -energy values for the two preferred slip systems. The DFT as well as the EAM results are shown in Fig. 3 (a) and (b). Owing to the reflection symmetry, only half of the energy curves are shown. Overall, the EAM γ -energies compare reasonably well to the DFT values, with typical differences less than 10%. The EAM results also reproduce the DFT stacking fault positions. Therefore, in the following we shall focus on EAM calculations only to provide trustworthy results within a reasonable computational cost. In Fig. 3(c), we display the projection of the lowest γ -energy surface for the (110) slip plane. Comparing to the one-dimensional γ -energy curves, the 3D projection can illustrate the topology of the γ -surface and reveal possible plastic deformation mechanisms. The preferential deformation mechanism would yield the lowest total energy, including both γ -energy and elastic energy of the system. One can estimate both energy contributions from the γ -surface. More specifically, two possible minimal energy paths are highlighted by the green and yellow curves in Fig. 3(c), starting and ending at the perfect crystal configuration. These two paths are obtained by tracing the gradient directions of the iso-energy surface, passing through the γ -energy troughs and connecting the stable stacking faults. For example, along the green path, the crystal undergoes deformations, encountering U1–S1–U2–S2–U3–S2–U2–S1–U1 stacking faults and returns to the perfect crystal configuration. Among the stacking faults, there are two *stable* stacking faults (S1 and S2) whose energies are 406 and 275 mJ m^{−2}, respectively, corresponding to the two local minima; there are three unstable stacking faults (U1, U2 and U3) whose energies are 484, 486 and 461 mJ m^{−2}, respectively, corresponding to local and global maxima. The global maximum U2 (486 mJ m^{−2}) along this path is much smaller than the energy barriers along [110] and [001] directions, which are 668 mJ m^{−2} and 538 mJ m^{−2}, respectively. Similarly, the yellow path also involves the stable stacking fault S2 and an unstable stacking fault U4 (538 mJ m^{−2}).

Based on the γ -surface, we speculate that the plastic deformation in Mg₁₇Al₁₂ may involve multiple partial or fractional dislocations along with complex stacking faults such as S1 and S2. However, since the stable stacking fault energies of S1 and S2 (406 and 275 mJ m^{−2}) are much higher than those of Mg (34 mJ m^{−2}) [23,22]

Fig. 3. The γ -energy curves for the two preferential slip systems as a function of the fractional displacement along (a) [110] and (b) [001] directions. The red and black curves represent DFT and EAM results, respectively. (c) Projection of the γ -surface on (110) plane. Two possible minimal energy paths are shown in green and yellow, with two stable stacking faults (S1 and S2) and four unstable stacking faults (U1, U2, U3 and U4). (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

and Al (164 mJ m^{−2}) [9], the partial dislocations would be rather narrow if exist. This speculation is in line with the well-known deformation mechanisms in many intermetallic compounds (such as transition metal aluminides) [24]. On the other hand, since the elastic energy of a dislocation is proportional to the square of its Burgers vector, a dislocation with a shorter Burgers vector would have a lower elastic energy. Taking the two energies into consideration, we predict that both the perfect dislocations with [001]-type Burgers vector and a combination of partial dislocations could be responsible for the plastic deformation of Mg₁₇Al₁₂ phase. However, the definitive conclusion would have to be drawn from direct experimental evidence (such as TEM images).

Recently, Wang et al. carried out DFT calculations to determine the elastic parameters of Mg₁₇Al₁₂ phase [19]. Based on the ratio of the shear modulus and bulk modulus, they concluded that Mg₁₇Al₁₂ phase was not brittle, contradicting to the experimental claims [5,25]. The reason for this contradiction could be the fact that the shear modulus alone is not a good indicator for the lattice

resistance to plastic deformation; likewise, the bulk modulus is not an accurate measure for the resistance to fracture. We believe that Rice's criterion on brittle-to-ductile transitions [26] is more appropriate and should be used instead for $\text{Mg}_{17}\text{Al}_{12}$. In Rice's model, the unstable stacking fault energy represents the lattice resistance to plastic deformation, and the surface energy (or Griffith fracture energy) measures the energy cost for a brittle fracture. The ratio between the surface energy and the unstable stacking fault energy indicates the tendency for a brittle fracture – the smaller the ratio, the more brittle the material. We have calculated the Rice ratio for the five slip systems of $\text{Mg}_{17}\text{Al}_{12}$ and the results are summarized in Table 1. The ratio ranges from 0.93 to 1.33 (EAM results), much smaller than the corresponding value of pure Mg (~ 6.14). As a comparison, we note that the ratio for Si (a prototypical brittle material) is 0.75, slightly smaller than the value of $\text{Mg}_{17}\text{Al}_{12}$. Finally, we have also performed molecular dynamics (MD) simulations for a crack in $\text{Mg}_{17}\text{Al}_{12}$ in an attempt to establish directly that $\text{Mg}_{17}\text{Al}_{12}$ is actually brittle. To this end, we focus on a crack whose slip system is of (110)[110] type. More specifically, the MD simulation domain has dimensions of $L_x \times L_y \times L_z = 300 \text{ \AA} \times 300 \text{ \AA} \times 20.8 \text{ \AA}$, where x ([1–10]) is along the crack propagation direction, y ([110]) is normal to the crack plane and z ([001]) is along the crack front. The crack was created by removing eight atomic planes at the crack tip. The crack was loaded with a constant velocity of $0.9 \text{ \AA/ps}$ along the y direction. We have run the MD simulation for 15 ps and observed a brittle fracture as shown in Fig. 4. Therefore, we conclude that $\text{Mg}_{17}\text{Al}_{12}$ phase is indeed brittle, consistent with the experimental evidence [5,25].

3.2. Mg dislocation interacting with Al particles and solid solution strengthening

In as-cast Mg–Al alloys and alloys with low Al contents, Al is dissolved into Mg matrix resulting in solid solution strengthening. Even at high Al contents, increasing temperature above 400 K could lead to the instability and dissolution of $\text{Mg}_{17}\text{Al}_{12}$ with Al particles formed in Mg matrix. The dissolved Al particles would

interact with dislocations and contribute to the strengthening of Mg–Al alloys. In the following, we study the energetics of Al particles interacting with the edge dislocation in the basal plane of Mg matrix, and quantify the solid solution strengthening effect due to the Al particles.

To simulate the interaction between an Al particle with the edge dislocation in Mg, we place the Al particle at the compressive region below the slip plane to minimize the elastic energy because the atomic radius of Al ($1.43 \text{ \AA}$) is smaller than that of Mg ($1.60 \text{ \AA}$). The typical dislocation core structure in the presence of the Al particle is shown in Fig. 5. The dislocation core is split into two partials with a stacking fault width of $5b$, consistent with the previous atomistic result [23]. In this case, the center of the Al particle is at a distance d from the right partial and is at the second atomic layer below the slip plane. These two quantities are used in the following to indicate the relative position between the dislocation and the particle.

We first examine the interaction between the dislocation and a single substitutional Al atom at the dislocation core with a supercell of $L=20$. Hence the neighboring Al atoms are separated by L along Z direction. In Fig. 6, we show the binding energy between Al and the dislocation as a function of the relative Al position. We find that there is a strong binding between them that gradually weakens as Al moves away from the dislocation. For the same d , the binding becomes stronger as Al approaches the slip plane.

Fig. 5. The schematic dislocation core structure in the presence of an Al particle. The two partials are labeled by the conventional symbol “T”. The position of the particle is defined relative to the right partial dislocation by the horizontal distance d . The vertical position of the particle is represented by the number of atomic layers below the slip plane.

Table 1
The surface energy γ_s , the unstable stacking fault energy γ_{us} and the ratio γ_s/γ_{us} for different slip planes and directions computed by EAM. For (110) plane, DFT results are available and included in the parenthesis. As a comparison, the corresponding values for pure Mg and Si calculated by DFT are also included. The unit of γ_s and γ_{us} is mJ m^{-2} .

Material	Plane	Direction	i	γ_s	γ_{us}	γ_s/γ_{us}
$\text{Mg}_{17}\text{Al}_{12}$	(100)	[100]	45	806	672	1.20
	(110)	[110]	145	716(662)	668(800)	1.07(0.83)
	(110)	[001]	145	716(662)	538(570)	1.33(1.16)
	(111)	[110]	5	790	785	1.01
	(111)	[112]	30	796	855	0.93
Mg [27]	{0001}	[1120]		540	88	6.14
Si [28,29]	(111)	[110]		1360	1810	0.75

Fig. 4. Atomic structure near the crack-tip region at (a) $t=0$ and (b) $t=15 \text{ ps}$ obtained from the MD simulations. The red arrow indicates the crack propagation direction. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

The interaction break-off distance is about $4b$, beyond which the binding energy quickly dies off. We have calculated the Peierls stress for the dislocation in the absence and the presence of Al. In the absence of Al, the Peierls stress is 17.9 MPa. In the presence of Al, the Peierls stress depends on its location at the dislocation core. When Al occupies the core center, the Peierls stress reduces to 11.3 MPa. When Al is located at the right partial, the Peierls stress is 14.6 MPa as the dislocation breaks away from Al, moving to the left. The Peierls stress is 19.2 MPa as the dislocation gets closer to Al, moving to the right. Hence a single Al atom at the dislocation core has a relative small effect on the Peierls stress (the Peierls stress at most increases 1.3 MPa).

Next we turn to two larger Al particles, one with a radius of 5 Å containing 19 Al atoms and the other with a radius of 10 Å containing 190 Al atoms. For each particle size, two different particle concentrations are considered corresponding to $L=20$ and $L=100$. The binding energy per Al atom between the Al particles and the dislocation is shown in Fig. 7. The left column displays the

Fig. 6. The binding energy (eV) between the dislocation and the substitutional Al atom. The Al atom resides at the first, second and fifteenth layer from the dislocation slip plane in the compressive zone. d is given in the unit of the Burgers vector.

Fig. 7. The binding energy for per Al atom (eV) between the dislocation and the Al particles: (a) the smaller ($R=5$ Å) and (b) the larger ($R=10$ Å) Al particle at the low particle concentration ($L=100$); (c) the smaller and (d) the larger Al particle at the high concentration ($L=20$). The particle center is indicated by d and the layer number below the slip plane. The lines are guide to the eye.

binding energy for the smaller Al particle at a lower particle concentration (top) and a higher concentration (bottom). The right column represents the binding energy between the larger particle at the lower particle concentration (top) and the higher concentration (bottom). The general trend of the binding energy is similar to that of a single atom, but with some important details due to the particle size effect. Comparing the two top panels for the lower concentration, we find that the smaller particle has a stronger binding per Al atom (a more negative energy) to the dislocation. And the same trend also holds for the higher particle concentration. The larger particle has a longer break-off distance ($12b$) than the smaller particle ($5b$). Hence the binding energy slope with respect to d at the break-off distance is much higher for the smaller particle – a fact that will be used to quantify the solid solution strengthening. For all cases, the binding is stronger if the particles are closer to the slip plane.

To better understand the interaction between the dislocation and the particles, we plot the averaged local strain field $\epsilon_i = (1/N_{nn})\sum_j(r_{ij}-r_{ij}^0)/r_{ij}^0$ [30] in Fig. 8. Here i and j are atomic indices and j sums over the nearest-neighbors of the atom i . N_{nn} is the number of the nearest-neighbors; r_{ij} and r_{ij}^0 represent the interatomic distances at the dislocated and the perfect lattice, respectively. To facilitate visualization, we render the dislocation core at the top plane of the supercell and the center of the particles at the front plane of the supercell; only half of the supercell is shown in Z direction owing to the symmetry.

The top row of Fig. 8 corresponds to the lower particle concentration in pure Mg (left), with the smaller particle (middle) and the larger particle (right). In the middle row, the same arrangements are displayed for the higher particle concentration. The partial dislocations are clearly visible in the dark-blue color and the original dislocation center is indicated by a dashed line. In all cases, the dislocation is attracted to the Al particles. The dislocation travels longer distances to the particles for the higher particle concentration. For the same particle concentration, the larger particle exerts a greater attractive force to the dislocation. The larger particle can lead to a constriction of the two partials. For a screw dislocation, such constriction would promote dislocation cross-slip and creep at high

Fig. 8. Local strain field around the dislocation core and the particles: (a) with no particle; (b) with the smaller particle at the lower concentration; (c) with the larger particle at the lower concentration; (d) with no particle; (e) with the smaller particle at the higher concentration; (f) with the larger particle at the higher concentration. The Hue change is assigned linearly with the strain from $+S$ to $-2S$. For (a), (b), (d) and (e), S is 0.03; and for (c) and (f) S is 0.045. (g) The atomic structure in the XOZ plane around the right partial as in the case of Fig. 8(e); (h) the atomic structure in the XOZ plane for the constriction as in the case of Fig. 8(f). The red and green circles denote Al and Mg atoms, respectively. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

temperatures. In Fig. 8(g) and (h), we also show the core structures corresponding to Fig. 8(e) and (f), respectively. The bending of the slip planes in Y direction is clearly visible in the case of the larger particle, reminiscent of the formation of a Frank dislocation. We have also estimated the Peierls stress (148 MPa) in the presence of the larger particle at the dislocation core ($L=20$). This Peierls stress is more than 8 times higher than that of pure Mg – a considerable strengthening owing to the changes of the core structure.

Next we carry out a simple elastic analysis to elucidate the elastic interaction between the dislocation and the particles. We assume that the particles are spherical with a radius R and they have dilatational misfit strains ($\epsilon_0 = -0.115$) [22] with respect to Mg matrix. We also assume that the elastic constants of the Al particles are the same as those of Mg to simplify the analysis. The dislocation would interact with these particles through their respective stress fields [31]. In particular, the stress field σ^p generated by the particle produces the Peach–Koeher force on the dislocation

$$\mathbf{F} = (\sigma^p \cdot \mathbf{b}) \times \boldsymbol{\zeta}, \quad (1)$$

where $\boldsymbol{\zeta}$ is the unit vector along Z .

In the following calculation, we place the Al particle at the origin, and the dislocation center is at (x, y, z) . Assuming isotropic elasticity, one can calculate the attractive force in X direction at (x, y, z) as [32,33]

$$F_X^p \approx -\frac{6\mu\epsilon b|xy|R^3}{r^5}, \quad (2)$$

where the particle–dislocation distance r is greater than R and μ is

the shear modulus (18.2 GPa). $\epsilon = \epsilon_0(1+\nu)/3(1-\nu)$ and the Poisson ratio $\nu = 0.29$; $r = \sqrt{x^2 + y^2 + z^2}$, $|x|$ is the X distance between the center of the particle to the dislocation core, and $|y|$ is the Y distance from the center of the particle to the slip plane.

We have calculated the two opposing forces on a given dislocation segment: the attractive force F_X^p and the lattice resistance force F_{latt} ; the latter is the product of the Peierls stress and the Burgers vector. Both forces are determined for a unit-length dislocation segment with F_X^p evaluated at $z=0$ and $|y|=R$. If $F_X^p > F_{\text{latt}}$, the dislocation would be attracted to the particles. Otherwise, the dislocation cannot translate although it may bow towards the particle. In Fig. 9, we show the ratio between the two forces (F_X^p/F_{latt}) as a function of d and R . For each particle, there is a critical d value below which the dislocation glides towards the particle, and above which the dislocation may only bow towards the particle but cannot glide. This critical distance is found to be $5b$ for the smaller particle and $12b$ for the larger particle; both are essentially the same as the corresponding break-off distance. In other words, the elastic interaction between the dislocation and the particles is primarily responsible for their binding energy. The larger particle has a longer critical and break-off distance as expected. Since F_X^p depends on z as $\sim z^{-5}$, the dislocation segment closer to the particle experiences a larger force than the distant segment. Therefore, the closer segment bends more severely or even glides towards the particle. In particular, at the higher particle concentration, the entire dislocation translates towards the particles as shown in Fig. 8(e) and (f). In contrast, at the lower concentration, the distant segment remains approximately straight

Fig. 9. The ratio of F_x^p and F_{latt} calculated at $z=0$ for the two particles ($R=5$ and 10 Å). d is given in terms of the Burgers vector.

Table 2

The maximum dislocation-particle interacting force F_{max} and the increase in CRSS $\Delta\tau$ for different particle sizes n and inter-particle distances L .

n	L	F_{max} (meV Å ⁻¹)	$\Delta\tau$ (MPa)
1	20	13.4	6.1
19	20	414.8	187.6
19	100	319.1	28.9
190	20	3034.7	1372.2
190	100	1260.9	114.0

and stationary as shown in Fig. 8(c). The shape of the dislocation line is determined by the balance between the line tension and the attractive force.

We can provide a quantitative estimate for the solid solution strengthening based on a model from Yasi et al. [22]. In this model, as a dislocation glides under stress, it encounters randomly distributed immobile precipitates (Al particles in this case). Each of the particles provides a pinning force up to the maximum dislocation-particle interacting force, F_{max} . F_{max} can be estimated by $\max |\vec{m} \cdot \nabla E_b(nAl, disl)|$, where E_b is the total binding energy and $\vec{m}$ is the Burgers vector direction. As alluded to earlier, $|\nabla E_b(nAl, disl)|$ corresponds to the maximum slope of the binding energy curves, multiplied by n . We have calculated the maximum slopes for five different cases, including a single Al atom, the smaller (and the larger) particle at the two particle separations, and the results are summarized in Table 2. At the critical bowing angle θ_c , F_{max} equals to $2\xi \sin((\pi - \theta_c)/2)$, where the line tension $\xi = 40 \text{ eV } e^{-1}$ [34] for the basal edge dislocation of Mg. We find that θ_c is slightly smaller than π , indicating that the Al particles can still be considered as weak obstacles. The solid solution strengthening, i.e., the increase in the critical-resolved shear stress (CRSS) at the basal plane necessary to overcome the solute attractive force, $\Delta\tau$ equals to $F_{max}/bL\sqrt{3}a_0$, depending on both F_{max} and the particle spacing at the basal plane, $L\sqrt{3}a_0$. For the singly dispersed Al solutes, our value of F_{max} is $13.4 \text{ meV } e^{-1}$, comparing well to that of Yasi et al. ($11.5 \text{ meV } e^{-1}$) [22]. For the solute spacing $L=20$, the calculated $\Delta\tau$ is 6.1 MPa which is a few times larger than the increase of the Peierls stress. However, this solid solution strengthening only amounts to $1/3 \sim 1/2$ of the Peierls stress. Since, according to Yasi et al., the solid solution strengthening is proportional to the product of $F_{max}^{3/2}$ and $C_s^{1/2}$ where C_s represents the concentration of solutes at the glide plane, it is plausible that the solid solution strengthening could overcome the Peierls stress at a higher solute concentration. On the other hand, for the larger particle examined here, $\Delta\tau$ (1372 MPa) is about 10 times greater than the corresponding Peierls stress (148 MPa) for $L=20$. We find

that relative to the singly dispersed Al solutes, the particles can provide up to 200 times increase in $\Delta\tau$ values. The larger particle at the higher concentration yields the greatest strengthening effect, while the smaller particle at the lower concentration renders the least strengthening.

4. Conclusions

In summary, we have studied two important problems underlying the plastic deformation of Mg–Al alloys using atomistic simulations. In the first problem, we investigate the possible plastic deformation mechanisms for the intermetallic phase $Mg_{17}Al_{12}$. Based on the analysis of the generalized stacking fault energy, we predict the preferential slip systems in this phase and speculate that the partial dislocations and complex stacking faults may be involved in the plastic deformation. Using the Rice's criterion, we confirm the intrinsic brittleness of the intermetallic phase. In the second problem, we simulate the interaction between the basal edge dislocation and dissolved Al particles. We have determined the binding energy between the dislocation and the particles and examined the energetic dependence on the particle size, particle separation and dislocation-particle distance. The strengthening effect due to the Al particles is characterized by two quantities – the Peierls stress and the solid solution strengthening factor; the former is due to the changes of the dislocation core structure while the latter is primarily due to the elastic interaction between the dislocation and the particles. For the larger particle, the latter plays a more important role than the former. The work provides a fundamental understanding of the plastic deformation and mechanical strength of Mg–Al alloys and offers insights that are not readily accessible to experiments but useful for the design of Mg–Al alloys.

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