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Effects of Alloying Elements on Stacking Fault Energies and Electronic Structures of Binary Mg Alloys: A First-Principles Study

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The growth, deformation, and extrinsic faults in binary Mg–X alloys are investigated via first-principles calculations. Here, the alloying elements X include Al, Ca, Cu, Fe, K, La, Li, Mn, Na, Nd, Pr, Si, Sn, Sr, Y, Zn, and Zr. In addition to stacking fault energies, the effect of the elements on the bond structure of Mg are studied in term of electron localization morphology. It is observed that rod-like directional bonds in non-fault planes transform into tetrahedral morphologies in fault planes and are strengthened by addition of Zn and Al, but weakened by Na.

Keywords: Magnesium Alloys, Alloying Elements, Stacking Faults, First-Principles Calculations

With a density that is two-thirds of aluminum or one-quarter of steel, Mg alloys are important structural materials for vehicles to improve fuel economy and reduce emissions.[1] The stacking fault energy, γ_{sf} , is an important property dictating deformation in Mg alloys.[2] It is closely related to the core structure and the mobility of the dislocations.[3–7] The reduction of γ_{sf} could enhance the twinnability of the material,[8,9] increase the ductility,[10–12] and reduce the steady-state creep rate.[13,14] The stacking sequence of an ideal HCP metal is ...ABABABAB... with A, B, (or C, see below) being different {0001} planes. There are three types of stacking faults commonly studied, i.e. growth fault (I1), deformation fault (I2), and extrinsic fault (EF). An I1 fault is formed by removing an A plane above a B plane, and then shearing the remaining planes above the B plane by $\frac{1}{3}[1\bar{1}00]$, resulting in ...ABA $\dot{B}$ CBCB... with the fault layer marked with a dot on top of it (same below). An I2 fault is formed by a shearing of $\frac{1}{3}[1\bar{1}00]$, resulting in ...ABA $\dot{B}$ CACA... [4,15] An EF fault is generated by inserting an extra C plane into the ideal HCP structure, resulting in ...ABA $\dot{B}$ C $\dot{A}$ BAB...

Recently, electronic structures have been used to gain insights into mechanical properties of materials.[16–19] For example, first-principles calculations based on density functional theory [20] indicate correlations between the elastic properties of Al, its bonding electrons, and the electrostatic potential distributions through the deformation electron density,[16] $\Delta\rho$, defined as the difference between the total electron density (ρ_{total}) and the electron density associated with unbounded atoms (ρ_{IAM}). In a previous work,[21] we found that the number of atomic layers affected by the presence of the stacking fault increases in the order of I1, I2, and EF in accordance with their stacking fault energies. Additionally, quantitative evaluations of charge density reveal that the redistribution range of deformation electron density along the [0001] direction is closely related to stacking fault energy.

Theoretical investigations of stacking fault energies of some binary Mg–X alloys have recently been reported in the literature [22–25] along with contour plots of electron density in 2D and electron density isosurface figures in 3D,[26–30] however, the detailed chemical bond structures of the fault and non-fault layers and the

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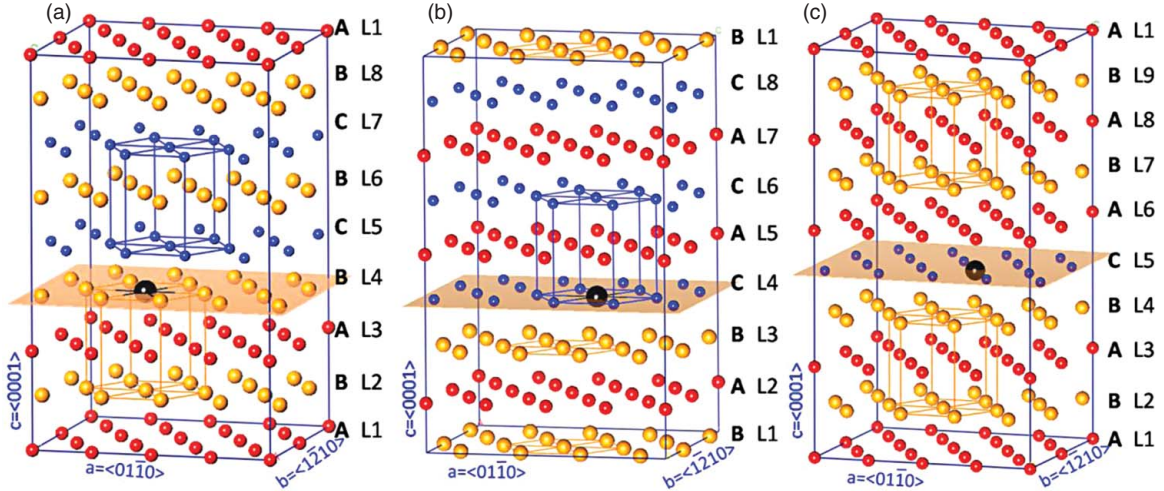


Figure 1. Schematic structure of the Mg–X alloys with different stacking faults (shown as (0001) miller plane), (a) growth fault—I1; (b) deformation fault—I2, and (c) EF. The atoms in different stacking layers are depicted with different color and size, with the alloying element being depicted as the largest size in the fault plane. The concentrations of the alloying element in fault planes are 6.25 at%.

contributions of alloying elements on the electronic structure of Mg with stacking faults have not been reported in the literature. In the present work, the effects of major alloying elements on the energies and bond structures of I1, I2, and EF of Mg–X alloys are systematically investigated through first-principles calculations in term of electron localization morphology. Based on their usage in advanced Mg alloys, the following alloying elements are included in the present study, i.e. Al, Ca, Cu, Fe, K, La, Li, Mn, Na, Nd, Pr, Si, Sn, Sr, Y, Zn, and Zr.

In the present first-principles calculations, the orthorhombic supercells of I1, I2, and EFs are designed as $4a' \times 2\sqrt{3}a' \times 4c'$, $4a' \times 2\sqrt{3}a' \times 4c'$, and $4a' \times 2\sqrt{3}a' \times 4.5c'$ with 128, 128, and 144 atoms, respectively, where a' and c' are the lattice parameters of primitive HCP Mg.[31] In Figure 1, the lattice vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ in the supercells are shown to be parallel to the directions of $\langle 01\bar{1}0 \rangle$, $\langle 1\bar{2}10 \rangle$, and $\langle 0001 \rangle$ of HCP Mg, respectively.

Calculations of stacking fault energy at 0 K are conducted by employing the Vienna *ab initio* simulation package [32,33] with the generalized gradient approximation (GGA) [34] for the exchange-correction functional and the projector-augmented wave [35] for the electron–ion interaction. The wave functions are sampled on the Γ -centered $5 \times 5 \times 3$ mesh. The plane wave cut-off energy is set as 1.4 times the default energy cut-off (ENCUT = 300 eV) and the energy convergence criterion of electronic self-consistency is 10^{-6} eV/atom. The structures are fully relaxed by the Methfessel–Paxton technique,[36] while the final total energy calculations are performed by the tetrahedron method incorporating Blöchl correction.[37] The total energies of I1, I2, and EF structures as a function of volume are fitted by a four parameters Birch–Murnaghan equation of state.[38]

From previously examined results looking at the effects of supercell size (on the $[0001]$ direction),[39] it was seen that the difference between three and seven atomic layers separating the stacking faults (I1, I2 and EF) is less than 3%. The deformation electron density,[16] $\Delta\rho$, is calculated using the Harris–Foulkes functional,[40,41] also known as the reference state in the independent atom model. The isosurface and the contour plots of the charge density are generated using VESTA.[42]

The stacking fault energy (γ_{sf}) is defined as

$$\gamma_{sf} = \frac{1}{A}(E_{sf} - E_{Bulk}) \quad (1)$$

where E_{sf} and E_{Bulk} are the total energies of supercells with and without stacking fault, respectively, and A the total area of the stacking fault planes. Due to the periodic boundary conditions used in our calculations, there are two identical interfaces in the I1 and I2 supercells and one in the EF supercell. Taking the stacking fault energy of pure Mg (γ_{sf}) as the reference, the segregation energy per area ($E_{seg}(X)$) is expressed as[43,44]

$$\begin{aligned} E_{seg}(X) &= \frac{[(E_{sf}(Mg_{n-m}X_m) - E_{sf}(Mg_n)) - (E_{Bulk}(Mg_{n-m}X_m) - E_{Bulk}(Mg_n))]/m}{A} \\ &= \gamma_{sf}(X) - \gamma_{sf} \end{aligned} \quad (2)$$

where $\gamma_{sf}(X)$ is the energy per area with alloying element in stacking faults, and m and n the number of solute atoms and the total number of atoms in the supercell.

Through the four parameters Birch–Murnaghan equation of state,[38] the total energies of I1, I2, and EF structures at equilibrium volume are obtained and

Table 1. First-principles calculated stacking fault energy (γ_{sf} , mJ/m²), and segregation energy per unit area of the dopants ($E_{seg}(X)$, mJ/m²) of Mg–X alloys with different structures at 0 K.

System	Growth fault (I1) Mg–0.78at%X		Deformation fault (I2) Mg–0.78at%X		Extrinsic Fault (EF) Mg–0.69 at%X	
	γ_{sf}	$E_{seg}(X)$	γ_{sf}	$E_{seg}(X)$	γ_{sf}	$E_{seg}(X)$
Mg	14.4 8.1–17.8 ^a , 11 ^b , 18 ^{c,d} , 16 ^e , 27 ^f , 22 ^f , 15 ^f , 17 ^{g,h} , 21 ⁱ	–	48.2 38.3 ^a , 33.8 ^c , 23 ^b , 33 ^d , 34 ^e , 54 ^f , 44 ^f , 30 ^f , 36 ^j , 34 ^{g,h}	–	99.3 80.6 ^g , 52.6 ^c , 36 ^b , 140 ^k , 59 ^e , 40 ^h	–
Mg–Al	12.5 13 ^d , 19 ⁱ	–1.8 –5 ^d , –3 ⁱ	33.6 23 ^d , 21 ^j	–14.6 –10 ^d , 16 ^j	55.7 130 ^k	–43.6 –10 ^k
Mg–Ca	13.8 12 ⁱ	–0.6 –9 ⁱ	33.5	–14.7	49.6	–49.7
Mg–Cu	16.6 23 ⁱ	2.3 2 ⁱ	41.0 53 ^j	–7.2 17 ^j	66.4	–32.9
Mg–Fe	3.3 (17.48 FM) 37 ⁱ	–11.1 (3.1) 16 ⁱ	40.3 (14.8 FM) 52 ^j	–7.9 (–33.4)	79.8 (119.0 FM)	–19.6 (19.7)
Mg–K	13.5 7 ⁱ	–0.9 –14 ⁱ	32.5	–15.7	47.5	–51.8
Mg–La	12.1 –3 ⁱ	–2.3 –18 ⁱ	24.7	–23.5	29.9	–69.5
Mg–Li	16.7 28 ^d , 23 ⁱ	2.3 10 ^d , 2 ⁱ	48.2 46 ^d , 47 ^j	–0.0 13 ^{d,j}	63.2	–36.1
Mg–Mn	13.5 33 ⁱ	–0.9 12 ⁱ	40.3 38 ^j	–7.9 2 ^j	81.4	–18.0
Mg–Na	15.7 18 ⁱ	1.3 –3 ⁱ	46.8	–1.4	66.7	–32.7
Mg–Nd	10.8 0 ⁱ , –2 ^h	–3.6 –21 ⁱ , –19 ^h	32.3 4 ^h	–15.9 –29 ^h	51.9 29 ^h	–47.4 –10 ^h
Mg–Pr	15.0 –1 ⁱ , –4 ^h	0.6 –22 ⁱ , –21 ^h	31.9 0.5 ^h	–16.3 –34 ^h	50.7 21 ^h	–48.6 –19 ^h
Mg–Si	13.8	–0.6	33.9	–14.3	50.5	–48.8
Mg–Sn	13.8 16 ⁱ	–0.6 –5 ⁱ	37.2 2 ^j	–11.0 –32 ^j	50.1 126 ^k	–49.2 –14 ^k
Mg–Sr	15.6 4 ⁱ	1.3 –17 ⁱ	33.2	–15.0	46.3	–53.0
Mg–Y	1.8 4 ^g , 5 ⁱ	–12.5 –13 ^g , –16 ⁱ	32.9 25 ^j , 16 ^g	–15.3 –11 ^j , –12 ^g	47.1	–52.3
Mg–Zn	8.5 18 ^g , 21 ⁱ	–5.9 1 ^g , 0 ⁱ	30.8 37 ^j , 35 ^g	–17.5 1 ^j , 1 ^g	58.8 18.9 ^l	–40.5 –61.7 ^l
Mg–Zr	9.8 13 ⁱ	–4.5 –8 ⁱ	35.3 26 ^j	–12.9 –10 ^j	67.5	–31.9

Note: Experimentally determined basal plane stacking fault energies of Mg are 78 mJ/m² [6] and ~50 mJ/m² [48]. The ferromagnetic (FM) moment of Fe atom is considered and listed in the brackets.

^aWang et al. first-principles calculation with GGA.[49]

^bChetty and Weinert first-principles calculation with Local density approximation (LDA).[4]

^cFan et al. first-principles calculation with GGA.[27]

^dHan et al. first-principles calculation of Mg–1.67at%X alloys.[28]

^eWen et al. first-principles calculation with GGA.[15]

^fHan et al. MD with different potentials.[28]

^gZhang et al. first-principles calculation of Mg–1at%X alloys with GGA and the concentration of alloying elements is ~11.1at% in the slip plane.[25]

^hZhang et al. first-principles calculation of Mg–2.08at%X alloys with GGA and the concentration of alloying elements is ~25at% in the slip plane.[24]

ⁱZhang et al. first-principles calculation of γ_{11} with GGA-Perdew-Burke-Ernzerhof (PBE) and the concentration of alloying elements is 11at% in the fault plane.[22]

^jMuzyk et al. first-principles calculation of Mg–2at%X alloys with GGA-PBE and the concentration of alloying elements is 25at% in the slip plane.[23]

^kWang et al. first-principles calculation of Mg–0.69at%X alloys with GGA and the stacking sequence is supposed to be ABACAB based on their cited literature by Datta et al.[50]

^lDatta et al. first-principles calculation of Mg and Mg–2.08at%X alloys with LDA.[30]

summarized in Table 1 along with various computational data in the literature with the majority of data for I1 from Zhang et al. [22] and those of I2 from Zhang et al. [24] and Muzyk et al. [23]. Correspondingly, the segregation behavior of the alloying element in stacking faults are obtained and shown in Figure 2. According to the crystal structures

of each individual solute atom at room temperature, it can be seen that some alloying elements with HCP and FCC structures reduce the stacking fault energies the most. If a reduction of stacking fault energies results in a high density of stacking fault, the strength can be improved without significant losses in ductility. [45,46] Thus, by

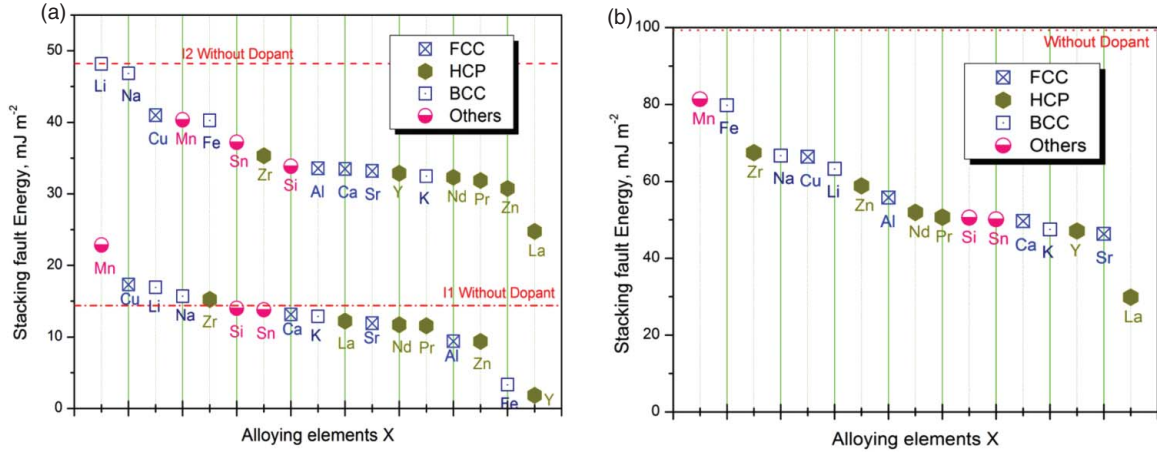


Figure 2. Contribution of alloying element on the formation energy of the basal plane stacking faults of binary Mg-X alloys, (a) Mg-0.78at%X alloys with growth (I1) and deformation (I2) faults; (b) Mg-0.69at%X alloys with EFs. Various symbols are used to identify the crystal structures of each individual solute atom at room temperature, such as FCC, BCC, HCP, and others.

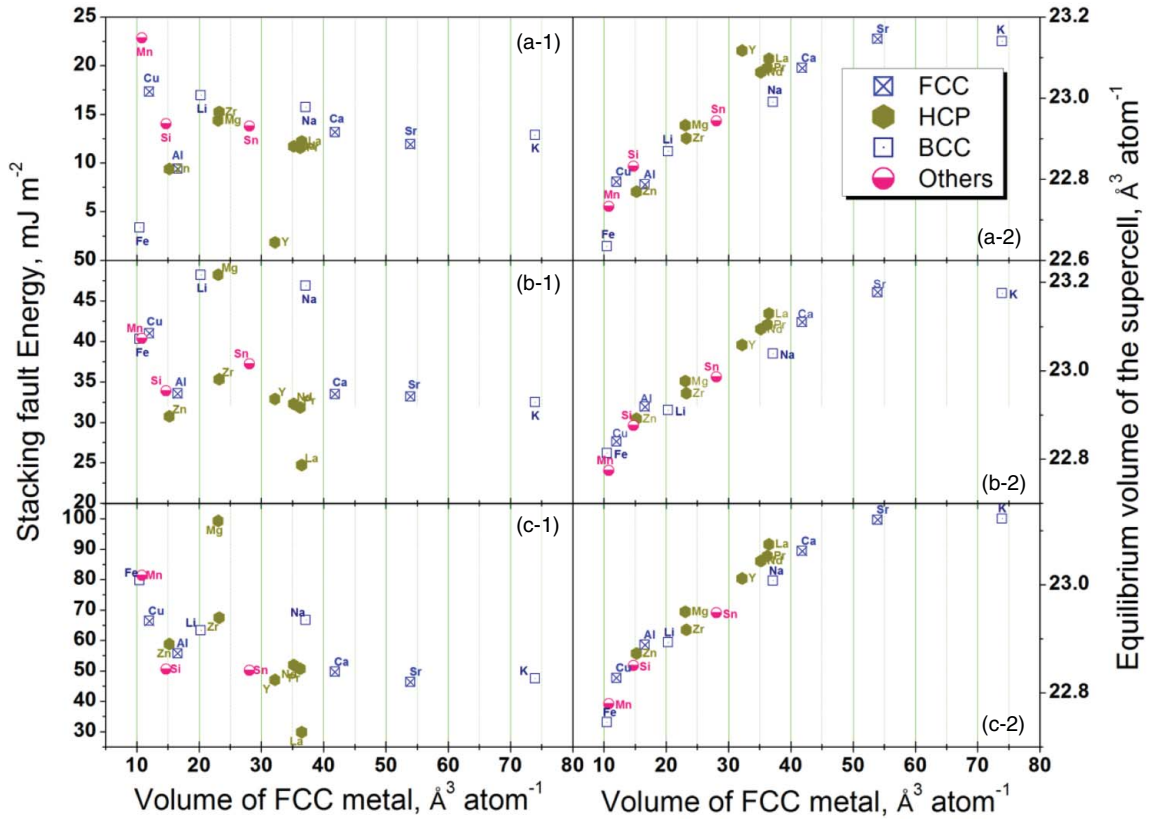


Figure 3. The calculated stacking fault energy and equilibrium volume of Mg-X alloys, referring to the alloying element X in FCC structure [31,38]; (a) growth fault, (b) deformation fault, and (c) EF. The numbers 1 and 2 are applied to characterize stacking fault energy and equilibrium volume in y-axis.

decreasing the width of Shockley partial dislocations in Mg,[6,47] the following alloying elements (La, Y, Zn, Al, Sr, Ca, Nd, and Pr) that are used in advanced Mg alloys are likely to be beneficial. It is noted that K reduces the stacking fault energies the most among all BCC alloying elements studied in the present work, probably due to its strong chemical reactivity.

It should be pointed out that the concentrations of alloying elements in a fault plane in the works by Muzyk et al. [23] and Zhang et al. [22,24] are 25 at% with all Mg atoms involved in Mg–X bonds and 11 at% with only one Mg–Mg bond, respectively, yielding strong interactions between alloying elements through X–Mg–X bonds in the fault plane. In the present work, the concentration

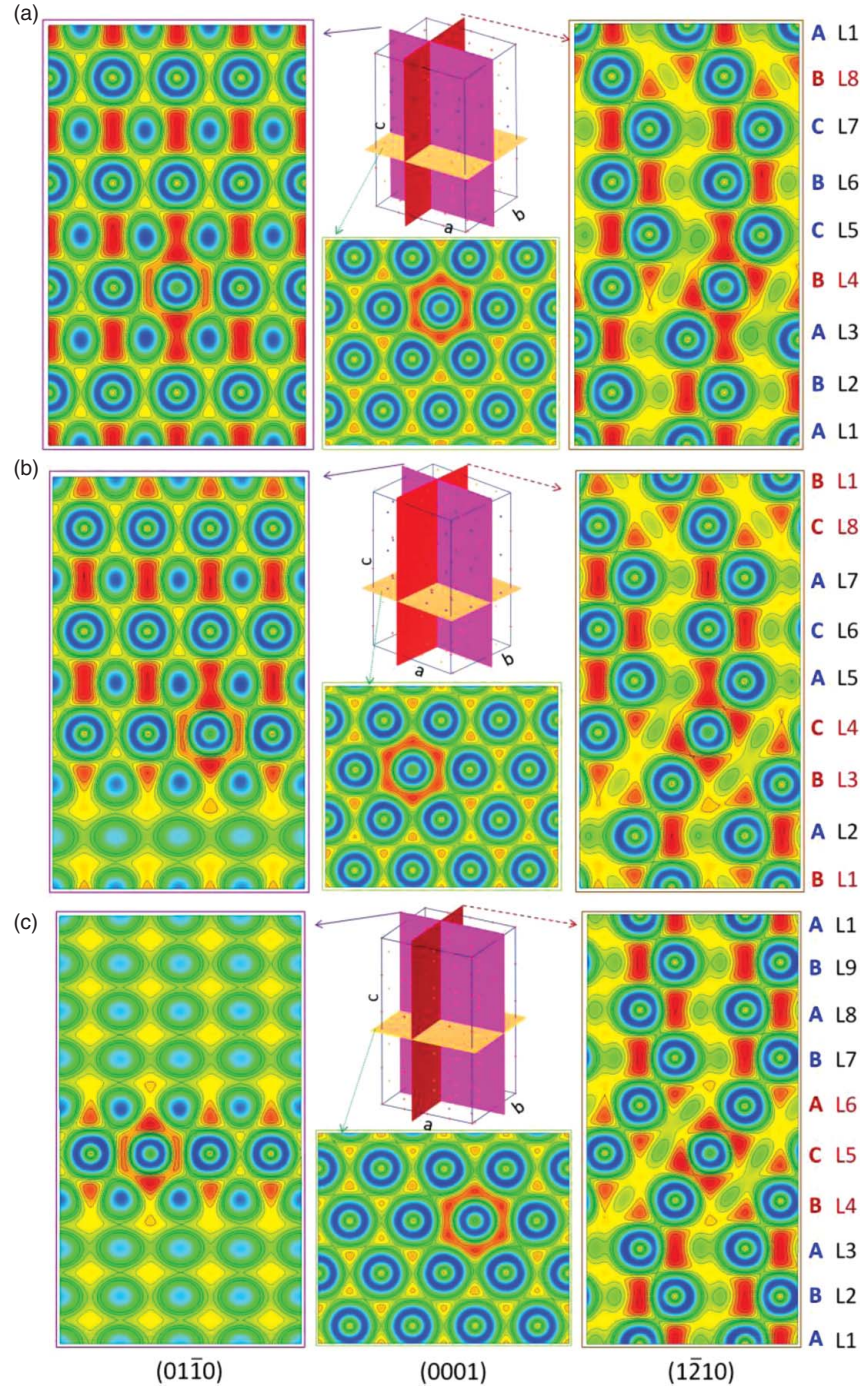


Figure 4. Contour plots of $\Delta\rho$ of Mg–Al in different views; (a) I1, (b) I2, and (c) EF with $0.0005 \text{ e}^-/\text{\AA}^3$ intervals. Plots are generated using VESTA [42] with red for $\Delta\rho > 0$ and blue for $\Delta\rho < 0$. The coordinates of each plane are identified by the corresponding Miller plane in the supercell.

of the alloying elements in the fault plane is 6.25 at% without the X–Mg–X bonds in the fault plane. The distance between two alloying element is larger than 11 Å to avoid the interaction between the elements.[39,51] The present setting is also in line with the experimentally determined concentrations of alloying element in the fault layers of Mg alloys, typically lower than 10 at% such as 2 ± 1 at%Zn– 4 ± 2 at%Y,[52] 7 at%Zn–6 at%Y,[53] 6 at%Zn–9 at%Y,[54] and 3 at%Zn–6 at%Y [53] in the alloys of Mg–1 at%Zn–2 at%Y. The different concentration of alloying elements is likely the reason for the discrepancy in reported data from Muzyk et al. [23] and Zhang et al.[22,24]

Since the local chemical environments for alloying elements in I1 (ABC), I2 (ACB), and EF (ACB) are similar to that of FCC, the calculated stacking fault energies and the Mg–X supercell volumes are plotted in Figure 3 with respect to the volume of each individual alloying element X in the FCC structure.[31,38] It can be seen that the equilibrium volumes of Mg–X supercells increase almost

linearly with the volume of alloying element X in the FCC structure. Consequently, it is plausible to select two alloying elements, both decreasing the stacking fault energy but changing the equilibrium volume in opposite way so that their co-segregation will be more energetically favorable due to the minimization of elastic lattice strain.[44]

In our previous study, isosurfaces of the deformation electron density (corresponding to $\Delta\rho_{\max}$) of I1, I2, and EF in pure Mg were used to study the effects of stacking faults and alloying elements on the bond structure.[21] It was observed that the shape of the $\Delta\rho_{\max}$ isosurface in fault planes is different from that in non-fault planes, and the number of atomic layers with altered electron density depends on the structure of stacking faults, i.e. 1, 2, and 3 for I1, I2, and EF, respectively. This indicates that the change of electron distribution is the largest for the EF and the smallest for I1 with that of I2 in between, in the same order as their stacking fault energies.

Figure 4 shows various contour plots of $\Delta\rho$ in I1, I2, and EF of the Mg–Al binary system. In the (1 $\bar{2}$ 10) plane

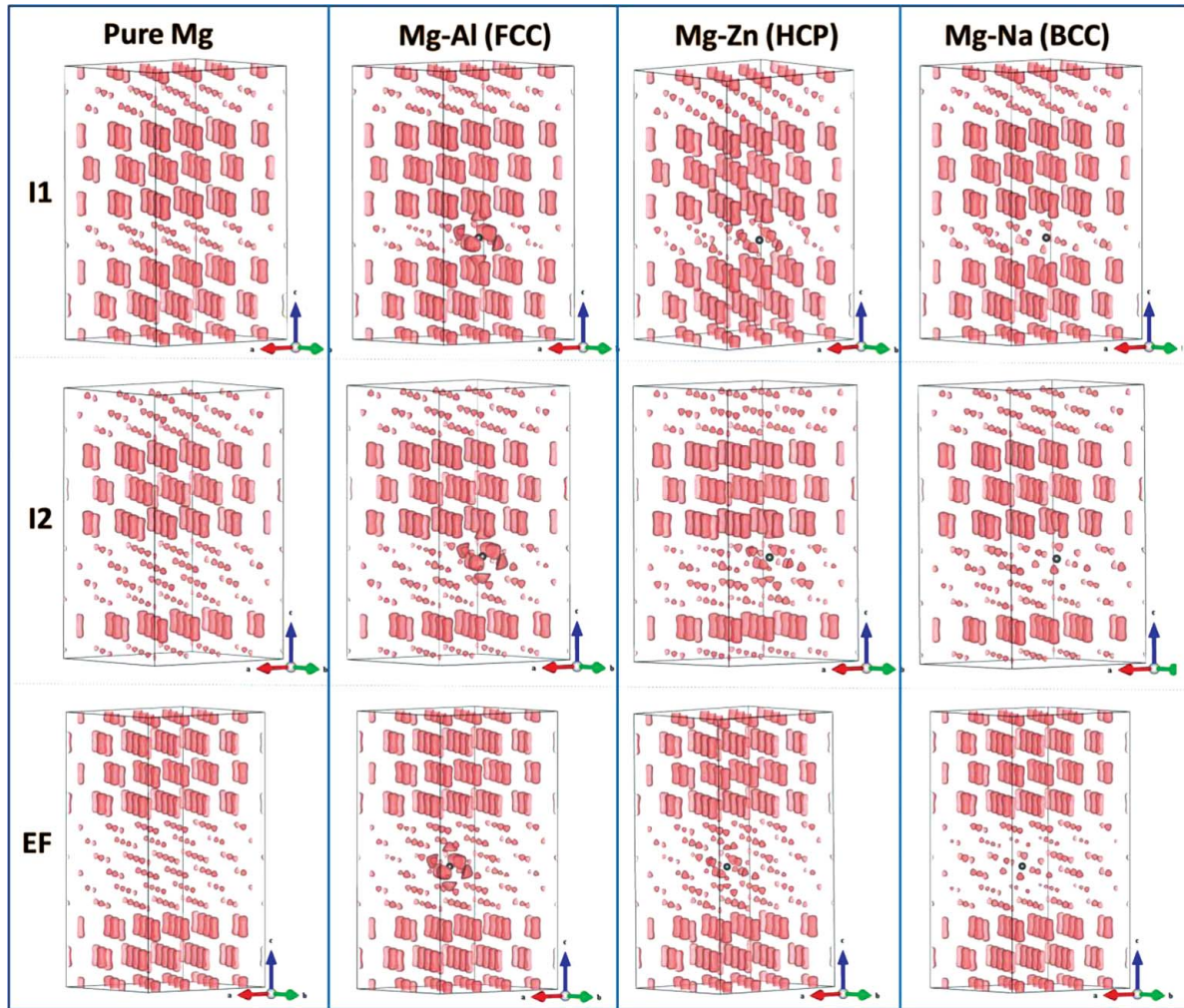


Figure 5. Deformation electron density isosurface ($0.75\Delta\rho_{\max}$) of Mg, Mg–Al, Mg–Zn, and Mg–Na with I1, I2, and EF (from top to bottom). Only alloying elements in the supercells are displayed in black.

view, the rod-shaped directional bonds within the non-fault planes match well with the previous investigation by Blaha et al., [55] while the triangle-shaped directional bonds are observed in the fault planes (L4 for I1, L3, and L4 for I2, and L4, L5, and L6 for EF). It can be seen that $\Delta\rho$ around the Al atomic basin has been increased compared with that without Al, i.e. Al and Mg atom in L5 of EF. In the (0001) plane view, $\Delta\rho$ around the Al atomic hexagonal basin is enhanced with respect to the case without Al, indicating the bond strength of basal plane is strengthened by Al. This is also consistent with the views of ($\bar{1}210$) and ($01\bar{1}0$) planes. Furthermore, the number of atomic layers with altered electron density around the Al atom is one non-fault planes for I1, one fault plane and one non-fault for I2, and two fault planes for EF as shown in Figure 4.

Figure 5 shows the $0.75\Delta\rho_{\max}$ (75% of the maximum value of $\Delta\rho$) isosurface of I1, I2, and EF with Al, Zn, and Na as alloying elements, respectively. It can be seen that the rod-like directional bonds have transformed into a tetrahedral shape with the addition of alloying elements in the fault plane. For alloying elements with the same crystallography structure, the similar electron localization morphology can be seen by plotting $\Delta\rho_{\max}$ isosurface. For example, the $0.75\Delta\rho_{\max}$ isosurface of I1, I2, and EF affected by FCC-Cu is similar to those of FCC-Al, shown as the second column of Figure 5. Moreover, the tetrahedral-shaped charge distributions in the fault planes are enhanced when alloyed with FCC-Al and HCP-Zn, see the second and third columns of Figure 5. On the contrary, the BCC elements show the reduced size of the tetrahedral-shaped charge distribution, for example, BCC-Na shown in the fourth column of Figure 5, agreeing with previous observations that Na reduces the bond strength in interfaces. [56,57]

In summary, the effect of 17 alloying elements on stacking fault energies of growth, deformation, and EFs in Mg is investigated through first-principles calculations. It is observed that all of them reduce the stacking fault energies of the deformation and EFs with La showing the least reduction for both. For the growth fault, five elements, i.e. Mn, Cu, Li, Na, and Zr, increase the stacking fault energy with the other elements decreasing the fault energy. As all stacking faults can be recognized as the local HCP-FCC transformation, the calculated results show that the bond strength is enhanced by alloying elements of FCC and HCP structures such as FCC-Al and HCP-Zn.

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