First-principles study of solid solution strengthening in Mg–X (X=Al, Er) alloys

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Abstract. To study the solid solution strengthening effect on magnesium (Mg)–X (X = Al, Er) alloys, supercell models of Mg, Mg₃₅Er and Mg₃₅Al are established to perform the first-principles pseudopotential plane wave calculations based on density functional theory. The calculated cohesive energy of Mg₃₅Er is lower than that of Mg₃₅Al. This indicates that Mg₃₅Er has better structural stability than Mg₃₅Al. The bulk modulus, Young's modulus and shear modulus of the solid solutions increases simultaneously when Al and Er are doped into the Mg matrix. Moreover, the solid solution strengthening of Er is much higher than the Al containing alloy. The order of toughness of the three solutions from the highest to the lowest is Mg, Mg₃₅Er and Mg₃₅Al, while the order of increasing elastic anisotropy is in the reverse order. The number of bonding electrons of Mg₃₅Er in the low-energy region of the Fermi level is much higher than that of Mg₃₅Al, and the density of states of Mg₃₅Er at the Fermi level is higher than that of Mg₃₅Al. Compared with Al atoms, Er atoms share more electric charges with Mg atoms, which leads to an increasingly uniform charge distribution around Er atoms.

Keywords. First-principles; Mg solid solution; solid solution strengthening; Er; Al.

1. Introduction

As the lightest structural metal, magnesium (Mg) alloys have many advantages such as low density, high-specific strength and stiffness, good machinability and excellent damping performance. These characteristics make Mg alloys increasingly applicable in the automotive, electronic communications, transportation and aerospace industries [1]. However, compared with Al, Fe and steel, the relatively poor mechanical properties and corrosion resistance of Mg alloys have seriously restricted their further application and development. Solid solution strengthening is one of the most effective methods to strengthen Mg alloys, because solute atoms can hinder the movement of dislocations owing to friction mechanisms, chemical interactions, short-range order and electrical interactions [2]. Although there are several studies on the solid solution strengthening effects of alloying elements on Mg alloys, the fundamental understanding of the solid solution strengthening mechanism at the atomic and electronic levels is still not clear. This understanding is very important for new Mg alloy research and development and is the focus of this work.

First-principles calculations based on density functional theory (DFT), which has attracted great attention from many researchers working on Mg alloys in recent years [2–4], is a method used to study material structures and properties through electron motion. Ganeshan calculated the lattice

parameters and elastic constants of Mg–X (X = Al, Ba, Ca, Cu, Ge, K, Li, Ni, Pb, Si, Y and Zn) solutions by first-principles calculations. The results revealed that large elements used as dopants in the alloy lead to an increase in the number of lattice parameters in Mg and the elastic properties of solute atoms play a key role in the elastic behaviour of Mg–X alloys [5]. Vassiliki studied the effects of Y and Zn atoms on the compressibility of Mg–X alloys using a simple thermodynamic model deduced by first-principles calculations. Their model estimated the bulk modulus of solid solutions in terms of the bulk moduli of the end members of the alloy [6]. Wu and Hu studied the solid solution mechanism of Mg_{100–x}RE_x (RE = Gd, Dy, Y, $x = 0.5, 1, 2, 3, 4$ at%) by molecular dynamics simulations, which showed that the bulk modulus of Mg alloys increased remarkably with the addition of Gd, Dy and Y. The addition of Gd leads to the most significant effect in which it sharply dropped the solid solubility with the decrease of alloy temperature [7].

Rare-earth elements are very important alloying elements in Mg alloys. The addition of a rare-earth element can refine grains, enhance mechanical properties and improve corrosion resistance. Er, which has an atomic radius of 1.757 Å, is a heavy rare-earth element in period VI and Group III of the Periodic Table. The lattice structure of Er is hexagonal close-packed (hcp), and its lattice parameters are $a = 3.560$ Å and $c = 5.595$ Å. The maximum solid solubility of Er in Mg is 32.7 mass% (6.56 at%), which leads to a higher solid solution

strengthening effect in Er containing Mg alloys compared with other dopants [8]. Rokhlin *et al* [9] found that by increasing the Er solution fraction up to 25% the strength of the Mg alloy at both room and elevated temperatures was improved and the ductility was still quite high.

In order to compare the effect of solid solution strengthening, the Mg–Al alloy is employed as a reference in this work. The supercell model of pure Mg and Mg_{35}X ($\text{X} = \text{Er}, \text{Al}$) solid solution is established to carry out the first-principles pseudopotential plane wave method based on DFT.

2. Computational model and method

2.1 Computational model

Mg has an hcp lattice with the space group $P63/mmc$ and two atoms in a unit cell. According to a report on the solid solubility of alloy elements at room temperature [5], a supercell comprising 36 atoms (35 Mg and 1 X atom, corresponding to 2.78 at% X) was modelled by a $3 \times 3 \times 2$ supercell of Mg (Mg_{36}), in which a Mg atom was replaced by a solute atom X ($\text{X} = \text{Er}, \text{Al}$). The crystal structures of Mg_{36} and Mg_{35}X ($\text{X} = \text{Er}, \text{Al}$) solid solutions are shown in figure 1.

2.2 Method

The Cambridge Serial Total Energy Package (CASTEP) based on first-principles DFT [10–12] was used in this study. CASTEP implements the plane-wave pseudo-potential (PWP) [13] in this work and we performed energy minimization using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) method [14,15]. The generalized gradient approximation of Perdew–Burke–Ernzerhof (GGA-PBE) was adopted to describe the exchange–correlation interactions [16]. An ultra-soft pseudo-potential presented in reciprocal space was used

for all elements in the calculation [17]. Monkhorst–Pack ($6 \times 6 \times 5$) k -points were sampled at the irreducible edge of the Brillouin zone [18]. An energy cut-off of 500 eV has been chosen for the plane-wave basis set for all calculations. This value is higher than the default cut-off energies for any elements. The relaxation of geometry optimization was performed until the total energy changes were within 2×10^{-5} eV per atom with the force on each atom lower than 0.5 eV nm^{-1} , the charge offset lower than 2.0×10^{-4} nm and the stress deviation lower than 0.1 GPa. The elastic stiffness constants of Mg_{36} and Mg_{35}X ($\text{X} = \text{Er}, \text{Al}$) at equilibrium volumes were obtained by the stress–strain method [19].

3. Results and discussion

3.1 Lattice parameters

Calculated and experimental lattice parameters of Mg and Mg–X ($\text{X} = \text{Er}, \text{Al}$) alloys are shown in table 1. The calculated lattice constant of pure Mg agrees with the experimental and calculated values in the literature [20–23]. This result shows the calculated lattice parameters a , c and the c/a ratio of Mg_{35}Er and Mg_{35}Al are reasonable.

As is shown in table 1, Mg lattice parameters a and c tend to decrease with the addition of 2.78 at% Al, while the c/a ratio exhibits a little increase. In the Mg–2.78Er alloy (at%), both the lattice parameters and c/a ratio are larger than those of pure Mg. The change of lattice parameters may be related to the radius of the solute atoms [5]. The addition of Al decreases the lattice parameters of Mg alloys because of the smaller radius of the Al atom, while the addition of Er increases the lattice parameters because of the larger radius of the Er atom.

Figure 1. Models of crystal cell for Mg_{36} and Mg_{35}X ($\text{X} = \text{Er}, \text{Al}$): (a) Mg_{36} ; (b) Mg_{35}Er ; (c) Mg_{35}Al . The light green sphere is Mg atom, the dark green sphere is Er atom, and the purple sphere is Al atom.

Table 1. Calculated and experimental lattice parameters of Mg and Mg–X (X = Er, Al) alloys.

Model		a (Å)	c (Å)	c/a
Mg	Present	3.196	5.181	1.621
	Ref. [20]	3.210	5.211	1.623
	Ref. [21]	3.210	5.211	1.623
	Ref. [22]	3.203	5.200	1.624
	Ref. [23]	3.209	5.211	1.624
Mg ₃₅ Er	Present	3.208	5.203	1.622
Mg ₃₅ Al	Present	3.187	5.183	1.626

Table 2. The total energy and cohesive energy of Mg₃₅X (X = Er, Al) solution alloys.

Model	Atomic number		E_{tot} (eV)	E_{coh} (eV per atom)
	Mg	X		
Mg ₃₅ Er	35	1	−39,316.578	−1.511
Mg ₃₅ Al	35	1	−34,143.827	−1.436

3.2 Cohesive energy

The stability of alloys directly affects the creep resistance, which is the key issue for the evaluation of alloy properties at elevated temperatures [24]. In order to study the stability of Mg₃₅X solid solution alloys, the cohesive energy is calculated as follows:

$$E_{\text{coh}} = \left(E_{\text{tot}} - N_{\text{A}} E_{\text{isolated}}^{\text{Mg}} - N_{\text{B}} E_{\text{isolated}}^{\text{X}} \right) / (N_{\text{A}} + N_{\text{B}}) \quad (1)$$

E_{tot} is the total energy of the supercell used in the present calculation, while $E_{\text{isolated}}^{\text{Mg}}$ and $E_{\text{isolated}}^{\text{X}}$ are the total energies of pure Mg and MgX (X = Er and Al) atoms in isolated states, respectively. N_{A} and N_{B} refer to the number of Mg and X (X = Er, Al) atoms, respectively. The calculated results are shown in table 2. The cohesive energy of pure Mg and Mg₃₅X (X = Er, Al) are all negative, meaning these three structures are all stable. The cohesive energy of Mg₃₅Er is lower than Mg₃₅Al which means Mg₃₅Er is more stable.

3.3 Elastic properties

3.3a Elastic constants: The elastic constant is an indicator of the anti-deformation ability of a material. Hooke's law is valid under small strains and the crystal energy E is a quadratic function of strain [25]. Hence, elastic constants can be calculated by applying small strains to the equilibrium unit cell and determining the corresponding variations in the total energy by first-principles methods. In the solutions for

a hexagonal symmetry crystal structure, there are only five independent elastic constants: C_{11} , C_{12} , C_{13} , C_{33} and C_{44} , since $C_{66} = (C_{11} - C_{12})/2$.

According to the Born stability criteria, the elastic constants must meet the following requirement [26]:

$$C_{11} > 0, \quad (C_{11} - C_{12}) > 0, \quad C_{44} > 0 \quad \text{and} \\ (C_{11} + C_{12})C_{33} - 2C_{12}^2 > 0. \quad (2)$$

As is shown in table 3, the calculated values of the elastic constants C_{ij} in Mg₃₅X (X = Er, Al) systems are very close to the theoretical and experimental values in the literature [5,27]. Additionally, all values obey formula (2) well indicating mechanical stability of Mg₃₅X (X = Er and Al) solution alloys.

Elastic constants C_{11} and C_{33} reflect the ability of the crystal to resist normal strain in the directions of the a and c axes, respectively. From table 3 and figure 2, it can be seen that the elastic constants C_{11} and C_{33} of Mg₃₅Al and Mg₃₅Er are larger than those of pure Mg. It is also shown that elastic constants C_{11} and C_{33} of Mg₃₅Er are the highest, which indicates that the addition of Er has the strongest effect on increasing the resistance of normal strain for Mg alloys. Elastic constants C_{44} and C_{66} reflect the ability of shear strain resistance in the directions of the a and c axes. The elastic constants C_{44} of Mg₃₅Al and Mg₃₅Er are slightly larger than that of pure Mg, which indicates that the addition of Al and Er can somewhat improve the resistance of shear strain in the direction of the a -axis. Moreover, compared with pure Mg, the elastic constants C_{66} of both Mg₃₅Al and Mg₃₅Er increase, and Mg₃₅Er has greater increase than the Mg₃₅Al solution. Thus, the appropriate addition of Al and Er into Mg can increase the shear strain resistance in the direction of the c -axis. Additionally, Er doping is more effective than Al containing solution.

3.3b Elastic modulus: The effective elastic moduli of polycrystalline aggregates are usually calculated using the average of single elastic constants in several schemes [28]. Voigt [29] and Reuss [30] approximation represents the maximum and minimum limits of the polycrystalline elastic modulus, respectively. The actual effective modulus can be approximated by the arithmetic mean of the two bounds, referred to as the Voigt–Reuss–Hill (VRH) value [30]. For the hexagonal system, the Voigt bounds of B and G are

$$B_{\text{V}} = \frac{2}{9}(C_{11} + C_{12} + \frac{1}{2}C_{33} + 2C_{13}) \quad (3)$$

$$G_{\text{V}} = \frac{1}{30}(7C_{11} - 5C_{12} + 12C_{44} + 2C_{33} - 4C_{13}). \quad (4)$$

And the Reuss bounds are

$$B_{\text{R}} = \frac{(C_{11} + C_{12})C_{33} - 2C_{13}^2}{C_{11} + C_{12} + 2C_{33} - 4C_{13}} \quad (5)$$

Table 3. The elastic properties of Mg and Mg₃₅X (X = Er, Al) solution alloys.

Material		C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B (GPa)	G (GPa)	E (GPa)	ν	G/B
Mg	Exp. [27]	59.5	25.9	21.8	61.6	16.4	16.8	35.6	17.3	44.6	—	0.48
	Present	60.59	23.29	22.28	57.78	12.46	18.65	35.47	15.72	41.09	0.31	0.44
Mg ₃₅ Er	Present	83.38	36.31	25.63	94.21	13.31	23.54	45.46	20.45	53.35	0.30	0.45
Mg ₃₅ Al	Present	63.72	24.88	19.68	69.61	13.36	19.92	36.57	18.58	47.67	0.28	0.51
	Calc. [5]	65.5	25.9	19.3	69.0	13.6	19.8	36.6	18.5	47.4	0.28	0.51

Figure 2. The values of C_{11} , C_{33} , C_{44} , C_{66} for Mg, Mg–Al and Mg–Er solution alloys. **Figure 3.** The values of elastic modulus for Mg, Mg–Al and Mg–Er solutions.

$$G_R = \frac{5}{2} \left\{ \frac{[(C_{11} + C_{12})C_{33} - 2C_{13}^2]C_{44}C_{66}}{3B_V C_{44}C_{66} + [(C_{11} + C_{12})C_{33} - 2C_{13}^2](C_{44} + C_{66})} \right\}. \quad (6)$$

The bulk modulus B and shear modulus G can be estimated using the VRH approximation using the following equations:

$$B = \frac{1}{2} (B_V + B_R) \quad (7)$$

$$G = \frac{1}{2} (G_V + G_R). \quad (8)$$

Furthermore, the Young's modulus and Poisson's ratio can be obtained by using the bulk modulus and shear modulus in the following equations:

$$E = \frac{9BG}{3B + G} \quad (9)$$

$$\nu = \frac{3B - 2G}{2(3B + G)}. \quad (10)$$

From table 3 and figure 3, we can see that the calculated bulk modulus B , shear modulus G , Young's modulus E , Poisson's

ratio ν and the B/G ratio of pure Mg agree very well with experimental and theoretical values in the literature [5,27]. This result indicates that our calculation has high reliability and accuracy. Compared with pure Mg, bulk modulus B , shear modulus G and Young's modulus E of the Mg solution alloys are all increased with the addition of Er and Al, especially for the case of Er addition. Therefore, Er has a larger influence than Al on the mechanical properties of Mg solution alloys.

3.3c Ductility:

(1) *Axial ratio* The ratio of c to a has been used to roughly estimate the ductile behaviour of hcp materials. A low axial ratio is associated with good isotropy and ductility. As is shown in table 1, the axial ratios of Mg, Mg₃₅Al and Mg₃₅Er are 1.621, 1.626 and 1.622, respectively. The axial ratios of Mg₃₅Al and Mg₃₅Er are larger than those of pure Mg, which means a lower ductility for Mg₃₅Al and Mg₃₅Er solutions. Compared with Mg₃₅Al, the axial

ratio of Mg_{35}Er is much closer to pure Mg, indicating that Mg_{35}Er still retains good ductility.

- (2) *Pugh's criterion* Pugh's criterion (the ratio of G/B) is reliable to analyse the toughness and brittleness of inter-metallic and solid solutions. When G/B is less than the critical value of 0.57, Mg alloys usually show good toughness [31]. The G/B values of pure Mg and Mg_{35}Er studied in this work are less than 0.57, which means pure Mg and Mg_{35}Er are both ductile materials. On the contrary, the G/B ratio of Mg_{35}Al is much higher than that of pure Mg, which indicates that the toughness of Mg decreased after the addition of Al.
- (3) *Poisson's ratio* Poisson's ratio (ν) is the ratio of transverse strain and longitudinal strain, and can also be used as a criterion for ductility/brittleness for many materials. Among all materials, the Poisson's ratios of air and water are the smallest ($\nu = 0$) and largest ($\nu = 0.5$), respectively, and the Poisson's ratio of all other materials is between these two values. The larger the Poisson's ratio, the better the material's toughness. The Poisson's ratios of Mg, Mg_{35}Er and Mg_{35}Al are shown in figure 4. The order of ν of the three solutions, from the largest to the smallest is Mg, Mg_{35}Er and Mg_{35}Al . Therefore, pure Mg is the toughest and Mg_{35}Al is the least tough. These results are in good agreement with results obtained earlier from the axial ratio and Pugh's criterion.

3.3d Anisotropy: The elastic anisotropy of a material is a very important technical index for engineering applications. The anisotropic behaviour of a non-cubic crystal system can be evaluated by the three following dimensionless parameters:

$$A_B = (B_V - B_R)/(B_V + B_R) \quad (11)$$

$$A_G = (G_V - G_R)/(G_V + G_R) \quad (12)$$

$$A_E = (E_V - E_R)/(E_V + E_R). \quad (13)$$

Figure 4. The values of G/B and Poisson's ratio ν for Mg, Mg–Al and Mg–Er.

Table 4. The calculated elastic anisotropy factor of Mg and Mg_{35}X ($\text{X} = \text{Er}, \text{Al}$) solutions.

Model	A_B (%)	A_G (%)	A_E (%)	A (%)
Mg	0.043	0.961	1.039	2.043
Mg_{35}Er	0.075	1.017	1.118	2.21
Mg_{35}Al	0.130	1.426	1.227	2.783

The subscripts V and R stand for the boundary of Voigt and Reuss, respectively. The calculated elastic anisotropy factor A ($A = A_B + A_G + A_E$) can be employed to assess the elastic anisotropy of a Mg solid solution. The calculated elastic anisotropy factor of Mg and Mg_{35}X ($\text{X} = \text{Er}, \text{Al}$) solutions is shown in table 4. These values decrease from Mg_{35}Al to Mg_{35}Er to Mg. Thus, micro-cracks are easy to initiate in Mg_{35}Al solution, and the Mg_{35}Al is the least tough.

3.4 Electronic properties

3.4a Density of state: The total electronic densities of states (TDOS) and partial electronic densities of states (PDOS) for Mg_{35}Al and Mg_{35}Er are shown in figure 5. The outermost electron configuration for the Al and Er atoms are $3s^23p^1$ and $4f^{12}6s^2$, respectively. As shown in the PDOS of the Al atom, the electrons of the S orbital determine the bottom belt, which is distributed from -7 to 3 eV. An obvious peak in the DOS of the S orbital is found in the low-energy bonding region (-7 to -6 eV), where two electrons of the S orbital are located. Electrons of the P orbital are mainly distributed around the Fermi level region (-6 to 3 eV), and the peak of the DOS can be seen around -2 to 0 eV. Hence, the DOS in the low-energy bonding region of the Fermi level are predominantly derived from the P orbital, which is the main orbital of bonding. Electrons in the high-energy region of the Fermi level are predominantly derived from the P orbital with a small contribution from the S orbital. As shown in the TDOS, the P orbital of Al and Mg will resonate and develop obvious orbital hybridization near the region of the Fermi level (-6 to 3 eV). Therefore, the Mg_{35}Al solution has a higher hardness and maintains certain plastic deformation ability.

As shown in the PDOS of the Er atom, the main DOS near the Fermi level is predominantly derived from the Er-4f orbital electrons. The peak of the DOS of Er-4f can be seen near -1 eV and Er-4f is the main bonding orbital in the low-energy bonding region of the Fermi level. The electrons of Er-4f also have a certain distribution in the high-energy bonding region of the Fermi level. Compared with the DOS of Mg, the addition of Er causes a clear pseudogap in the TDOS. The Fermi level is at the low-energy region of the pseudogap, where electrons are able to easily transit, leading to good metallicity and ductility. Compared with the TDOS of the solid solution of Mg_{35}Al , the quantities of bonding electrons of Mg_{35}Er are more than Mg_{35}Al at the low-energy region of the Fermi level. The atomic interaction of the Mg_{35}Er solution

Figure 5. Total and partial density of states for (a) Mg_{35}Al and (b) Mg_{35}Er .

Figure 6. The difference charge density map on (110) plane of (a) Mg_{35}Al and (b) Mg_{35}Er .

is stronger, which leads to a greater deformation resistance. The DOS of Mg_{35}Er is higher than that of Mg_{35}Al in the Fermi level region, indicating that Mg_{35}Er has the better metallicity and ductility.

3.4b Difference charge densities: The difference charge density map on the (110) plane of Mg_{35}Al and Mg_{35}Er is shown in figure 6. The charge densities are represented by different colours. Blue, red and white represent the regions of the gain electrons, loss electrons and intermediate state, respectively. The amount of shared electrons between Er and Mg atoms is more than that of Al and Mg atoms resulting in a stronger covalent bond between Er and Mg atoms. Compared with the distribution of charges around an Al atom, the distribution of electrons around an Er atom is more uniform and has less directionality. Compared with the doped Al atoms, the doped Er atoms not only increase the elastic modulus of the Mg solution, but also maintain a good isotropy and ductility.

4. Conclusion

- (1) The Al dopant decreases the lattice parameters of the Mg solution, while the Er dopant increases the lattice parameters of the Mg solution. The calculated cohesive energy of Mg_{35}Er is more negative than that of Mg_{35}Al which means Mg_{35}Er has the highest stability.
- (2) The elastic constants of Mg_{35}Al and Mg_{35}Er show improvement compared with pure Mg and the elastic constant of Mg_{35}Er shows the highest improvement. For Mg doped with Al and Er, the bulk modulus (B), Young's modulus (E) and shear modulus (G) of the solid solution all increased and the solid solution strengthening effect of Er is much greater than Al. The calculated results of c/a , G/B , Poisson's ratio and the anisotropy factor show that the toughness from largest to smallest is Mg, Mg_{35}Er and Mg_{35}Al . The order of elastic anisotropy for the three solutions is reversed from that of the toughness.

- (3) The quantity of bonding electrons of Mg_{35}Er is greater than Mg_{35}Al at the low-energy region of the Fermi level. The atomic interaction of the Mg_{35}Er solution is stronger, which leads to a greater deformation resistance. The DOS of Mg_{35}Er is higher than that of Mg_{35}Al in the Fermi level region, which indicates that Mg_{35}Er has the better metallicity and ductility. The amount of shared electrons between Er and Mg atoms is much more than that between Al and Mg atoms, which result in a stronger covalent bond between Er and Mg atoms. Compared with the distribution of charges around an Al atom, the distribution of electrons around an Er atom is more uniform and demonstrates less directionality.

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