Mechanical Properties of Al–5 wt%Mg from First Principles Study

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(Received November 23, 2017; in final form September 14, 2018)

We have investigated the mechanical properties of Al–5 wt%Mg using the first-principles method. The elastic constants, shear modulus, Young's modulus, Poisson's ratio and the brittle/ductile characteristics of Al–5 wt%Mg are successfully obtained. The stress-strain relations and ideal strengths under tension and compression loading of Al–5 wt%Mg have also been determined. Results show that Al–5 wt%Mg is found to have larger moduli and higher strengths than Al, which is consistent with its exploitation in Al precipitate-hardening mechanisms. The electronic structure is investigated to unveil the intrinsic mechanism for the mechanical properties of Al–5 wt%Mg. It turns out that the partly covalent-like bonding through Al p–Mg s hybridization is the origin of excellent mechanical properties of Al–5 wt%Mg. We expect that the present work should be helpful to the performance of Al–5 wt%Mg.

DOI: 10.12693/APhysPolA.134.1115

PACS/topics: Al–5 wt%Mg, mechanical properties, first principles, stress– strain relations, ideal strength

1. Introduction

The mechanical properties of a material have been studied by both first-principles calculations and experimental methods. One fundamental measure of the mechanical strength of a material is its ideal strength. The ideal strength describes the mechanical properties of the material beyond the linear region. The ideal strength sets an upper bound on the attainable stress at which a perfect crystal becomes mechanically unstable. Experimental observations on ideal strength are scarce because it is difficult to measure the ideal strength using experimental tools. The ideal strength is one of few mechanical properties that can be calculated from first principles. Therefore, theoretical investigations into the ideal strength are of great importance because they represent an upper limit to the strength of a real crystal. The ideal strength may be calculated in terms of tensile strength and compressive strength with corresponding applied loads. The ideal tensile strength is when a material becomes unstable with respect to fracture by the spontaneous separation of atomic planes. The ideal compressive strength describes the pressure limit of a material through uniaxial compression.

Currently, alloys of Al is one of the most widely used structural materials. Al–Mg alloys are candidates for components that require moderate strength, formability, and weldability. Investigations show that adding up to 10% of magnesium of aluminum increases its strength, while retaining the low density of Al [1]. Alloy AA5456 is an Al–Mg alloy with a nominal concentration of 5 wt%Mg, which meets these goals. Therefore in this paper, a single phase Al–5 wt%Mg embedded in the ordered α Al solid-solution matrix is investigated. Al–5 wt%Mg is often used to deliver a broad range of specific property requirements, such as aircraft and automotive industries etc. The crystal structure of Al–5 wt%Mg is face-centered-cubic structure with the space group Fm-$3m$ (No. 225) [2]. To the binary Al–Mg system, an extensive amount of experimental and theoretical data, such as phase equilibria, crystal structures of solid phases, and thermodynamic properties etc., have been reported in previous work [3–5]. For constituent element of Al–Mg system: fcc Al, several theoretical studies of the ideal strengths have appeared [6–10]. However, the experimental and theoretical investigations of ideal strength of Al–5 wt%Mg are rather limited. In this work, we use the reliable first-principles methods based on density functional theory (DFT) to investigate the ideal strength of Al–5 wt%Mg. The primary purpose of our work is to give the ideal tensile strength and compressive strength of Al–5 wt%Mg. Second, we aim to gauge the relative significance of Mg atom in the mechanical properties of Al–5 wt%Mg.

To understand the mechanical behavior of Al–5 wt%Mg, we first estimate its elastic properties. The elastic parameters describe the mechanical properties of a material in the region of small deformations where the stress-strain relations are still linear. Then we investigate the stress-strain relations under uniaxial tensile and compressive deformations. The strength and ductility at large strains would also be estimated. The combination of elastic parameters and ideal strength will be used to fully access the mechanical properties of Al–5 wt%Mg. For comparison we have performed the same study for fcc Al. As the structure of Al–5 wt%Mg is also an fcc structure, it is possible to compare the results directly with fcc Al.

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This paper is organized in the following way. In Sect. 2 we present the computational details. In Sect. 3, we first give the lattice constant of Al–5 wt%Mg. Secondly, we assess the accuracy of our calculations on the mechanical properties by considering pure Al. Thirdly, we study the elastic constants and the ideal strengths of Al–5 wt%Mg. Finally, the conclusions are summarized in Sect. 4.

2. Computational details

Our calculations have been carried out using the Vienna *ab initio* simulation package (VASP) [11], which is based on first-principles density functional theory (DFT) and the projector augmented wave method [12]. The generalized gradient approximation (GGA) [13] within the Perdew–Wang scheme (PW91) exchange-correlation functions is adopted in our calculations. We use a 4 atom conventional cell for calculations of the pure Al bulk properties. The electron wave function is expanded in plane waves up to a cutoff energy of 350 eV and the Monkhorst–Pack $24 \times 24 \times 24$ mesh is used in the Brillouin zone (BZ) integration. A $2 \times 2 \times 2$ supercell which includes 30 Al atoms and 2 Mg atoms is employed for our calculations on Al–5 wt%Mg. A kinetic energy cutoff of 350 eV and $7 \times 7 \times 7$ k-mesh are chosen to achieve the convergence of calculated total energy. In order to determine whether the number of different atoms will affect the mechanical properties of Al–5 wt%Mg, a $3 \times 3 \times 3$ supercell which includes 102 Al atoms and 6 Mg atoms is also performed. A 350 eV cut-off energy is chosen and $3 \times 3 \times 3$ k-mesh is used in the calculation of 108-atom supercell. Figure 1 shows the crystal structure of Al–5 wt%Mg.

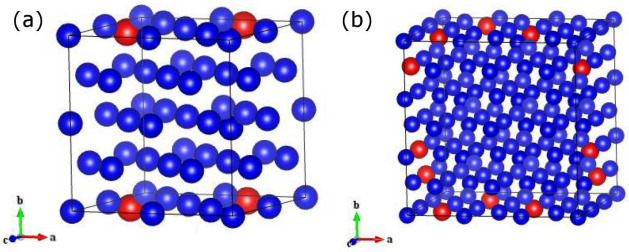

Fig. 1. (a) A 32-atom supercell and (b) a 108-atom supercell of Al–5 wt%Mg. Red (big) balls represent Mg atoms and blue (small) balls represent Al atoms.

The elastic properties are evaluated by the stress-strain method [14]. According to this method, appropriate strains of ± 0.002 are applied to determine the corresponding variation of total energy, and then elastic constants are obtained by fitting the energy–strain curves. The calculation approach to determine the ideal strength was described in detail previously [15, 16]. The lattice vectors are deformed incrementally in the direction of the applied strain with an interval of 0.02. At each strain, we relax the deformed structure to make sure that all of the components of the Hellmann–Feynman stress tensor orthogonal to the applied stress are less than 0.1 GPa. To ensure continuity of the strain path, the starting atomic positions at each strain step are taken from the relaxed cell of the previous strain step. The tensile stress σ and the shear stress τ are, respectively, calculated from Eqs. (1) and (2) [17]:

$$\sigma = \frac{1}{V(\varepsilon)} \frac{\partial E}{\partial \varepsilon}, \tag{1}$$

$$\tau = \frac{1}{V(\gamma)} \frac{\partial E}{\partial \gamma}, \tag{2}$$

where E is the total energy, $V(\varepsilon)$ and $V(\gamma)$ are the volumes at the given tensile strain ε and shear strain γ, respectively.

3. Results and discussions

3.1. Elastic properties

Our calculations start with the structural optimization by minimizing the total energy to obtain the equilibrium lattice constant in the ground-state structure. Experimental work by Mondolfo [2] revealed that the lattice constant of Al increases about 0.005 Å with Mg content increasing by 1% in Al–Mg solid solution. Our calculated equilibrium lattice parameters are 4.074 Å and 4.067 Å for the 32 and 108 atom supercells of Al–5 wt%Mg. The deviation is only 0.007 Å for the 32 and 108 atom supercells, indicating that the effect of different supercells on the structural optimization is small. The value $a = 4.075$ Å given by Mondolfo [2] is slightly larger than our values of $a = 4.074$ Å. It indicates that the structural properties are reproduced well and the results are largely sufficient to study the mechanical properties.

Then we calculate the elastic parameters to describe the mechanical properties of Al–5 wt%Mg in the region of small deformations. For cubic symmetry, there are only three independent elastic constants c_{11}, c_{12}, and c_{44}. As a test, we have calculated the elastic constants of pure Al. All elastic constants are listed in Table I. For Al, the overall agreement of our calculated values and experiment is satisfactory. These results indicate that our computational approach is reliable. From Table I, the elastic parameters for the 32 and 108 atom supercells vary little, which indicates that the effect of different supercells on the elastic properties is also small. We examine the mechanical stability of Al–5 wt%Mg according to the stability condition for cubic lattice as the following restrictions [18]:

$$c_{44} > 0, \quad c_{11} > |c_{12}|, \quad c_{11} + 2c_{12} > 0. \tag{3}$$

From Table I, our calculated elastic constants meet the above criteria, indicating that Al–5 wt%Mg is mechanically stable.

Based on the calculated elastic constants, the elastic modulus of polycrystallines can be further obtained from the Voigt formalism: the bulk modulus $B = (c_{11} + 2c_{12})/3$, the shear modulus $G = (c_{11} - c_{12} + 3c_{44})/5$, Young's modulus $Y = 9BG/(G+3B)$ and Poisson's ratio $\sigma = (B - 2G/3)/(2B + 2G/3)$. These calculated results

TABLE I

The calculated elastic properties of Al and Al–5 wt%Mg, the experimental results are also listed for comparison. G is shear modulus in GPa, Y is Young's modulus in GPa, σ is Poisson's ratio, and G/B is ratio between shear modulus and bulk modulus.

System	c_{11}	c_{12}	c_{44}	G	Y	σ	G/B
Al	101.8	60.2	28.2	25.2	67.9	0.35	0.34
Exp[a]	108.0	62.2	28.4	26.0	70.0	0.35	0.37
Al–5 wt%Mg ($Al_{30}Mg_2$)	108.8	54.1	29.7	28.8	76.1	0.32	0.40
Al–5 wt%Mg ($Al_{102}Mg_6$)	104.1	54.8	29.1	27.3	72.6	0.33	0.38

[a]Ref. [19]

are summarized in Table I. Obviously, the elastic properties of Al–5 wt%Mg are similar to that of Al, which can be attributed to the fact that Al and Al–3 wt%Mg have the same fcc structure. It is well-known that Young's modulus and shear modulus are two of several quantities for measuring the stiffness of a solid material. The material is stiffer for larger Young's modulus and larger shear modulus. From Table I, Al–5 wt%Mg has larger shear modulus and Young's modulus in contrast with Al. It can be judged that Al–5 wt%Mg is a harder material, consistent with its exploitation in Al precipitate-hardening mechanisms. According to Pugh's empirical rule [20], we can evaluate the ductile/brittle nature of a material. The G/B value of 0.57 is commonly regarded as a value to separate the ductile and brittle material. Our calculated value of G/B for Al–5 wt%Mg is below 0.57, indicating that Al–5 wt%Mg should be regarded as a ductile material. One should be aware that Poisson's ratio can describe the stability of a crystal against shear to some extent [21]. Our calculated Poisson's ratio of Al–5 wt%Mg is smaller than 0.5, which indicates that Al–5 wt%Mg is relatively stable against shear. Based on the rule that $\sigma = 0.25$ is the lower limit and 0.5 is the upper limit for central-force solids [21], the interatomic forces in Al–5 wt%Mg are central. Overall, the structural and elastic properties are reproduced well in these two supercells for Al–5 wt%Mg. To save computing resources and times, we mainly use the 32 atom supercell to investigate tensile and compressive properties in the following sections.

3.2. Ideal tensile strength

To obtain a deep insight into the intrinsic mechanical properties of Al–5 wt%Mg, We impose a tensile strain on the Al–5 wt%Mg crystal. The strains are imposed in the high-symmetry ⟨100⟩, ⟨110⟩ and ⟨111⟩ directions common for cubic crystals. The stress–strain curves of Al–5 wt%Mg under tensile loading are plotted in Fig. 2. Figure 2 shows that the stress–strain curves of Al–5 wt%Mg coincide in the original stage in spite of the different tensile paths. The phenomenon reveals that Al–5 wt%Mg has rather isotropic Young's modulus for different crystal directions. The behavior is nearly identically to fcc Al, which indicates that the underlying crystal structure is the most important factor in the uniaxial tensile deformation.

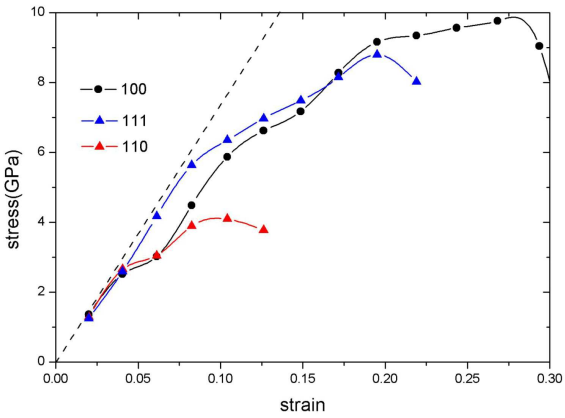

Fig. 2. The stress-strain relationships of Al–5 wt%Mg under tension loading.

TABLE II

The ideal strengths and critical strains of Al and Al–5 wt%Mg under tensile loading.

System	Loading configuration	Ideal strength [GPa]	Critical strain	Reference
Al	⟨100⟩ tension	11.33	0.345	this work
		12.92	0.340	Ref. [6]
	⟨110⟩ tension	4.13	0.126	this work
		4.92	0.140	Ref. [6]
	⟨111⟩ tension	9.80	0.319	this work
		11.30	0.330	Ref. [6]
Al–5 wt%Mg	⟨100⟩ tension	9.76	0.268	this work
	⟨110⟩ tension	4.20	0.149	this work
	⟨111⟩ tension	8.80	0.195	this work

The first maximum stress in the stress–strain curve is the ideal strength, the strain corresponding to the ideal strength is called critical strain. The calculated ideal tensile strengths and critical strains of Al and Al–5 wt%Mg are listed in Table II. We note that our results of Al for stress are by about 10%–20% lower than the values given by Clatterbuck et al. [6]. It must be pointed out that Clatterbuck et al. [6] Obtained their results using the local density approximation (LDA) [22–24] and we perform our calculations using the GGA. It is known that the LDA produces strengths 10%–20% higher than GGA [10]. For critical strain, our values can be compared with the results given by Clatterbuck et al. [6]. From the above findings, we conclude that our computational approach has high accuracy in describing the uniaxial tensile deformation of Al and thus can be further employed to investigate the uniaxial tensile deformation of Al–5 wt%Mg.

From Fig. 2, we can observe a short region of a linear behavior near the origin. Young's modulus is related to the slope of the linear part of the stress–strain curve near the origin. It is represented by the dotted straight lines in Fig. 2. The value of Young's modulus of $Y = 76.9$ GPa extracted from the linear region agrees well with the value $Y = 76.1$ GPa calculated from the elastic constants. The agreement is also a good check for our calculations.

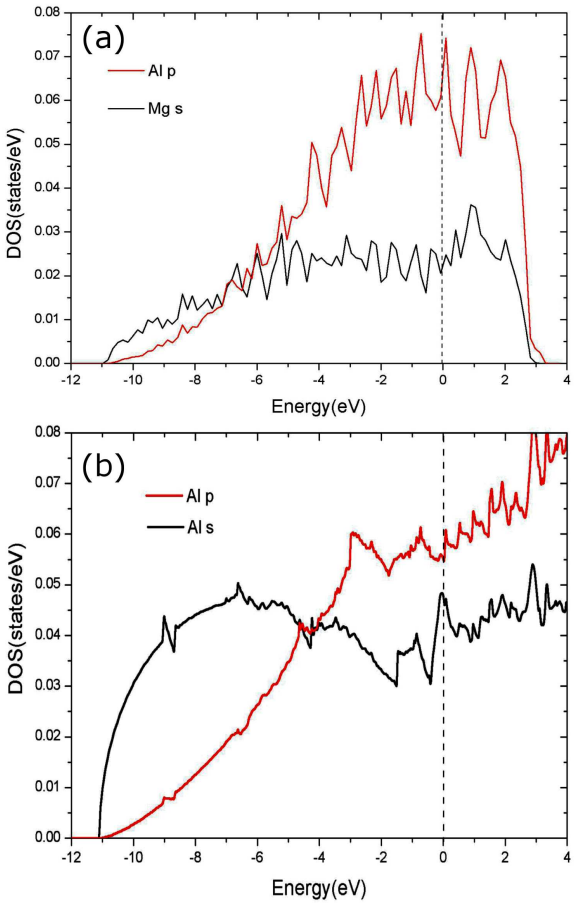

Fig. 3. (a) The PDOS for the Al p and Mg s of Al–5 wt%Mg; (b) The PDOS for the Al p and Al s of Al. The vertical dashed line indicates the Fermi level.

In general, the tensile strength in the easiest tensile direction is thought to be the ideal tensile strength. Since the value of the ideal tensile strength along ⟨110⟩ direction is the lowest, ⟨110⟩ is the easiest tensile direction for Al–5 wt%Mg. Therefore the ideal tensile strength of Al–5 wt%Mg is 4.20 GPa, which is higher than that of pure Al. It results from the strength of Al–Mg bonding which lies mainly through the ⟨110⟩ crystal direction. Al–5 wt%Mg has a higher tensile strength, which is consistent with its exploitation in Al precipitate-hardening mechanisms and indicates a bright applicable prospect of Al–5 wt%Mg. In reality, the mechanical properties of a material is closely related to its internal electronic structure. We plot the partial density of states (PDOS) of Al and Al–5 wt%Mg in Fig. 3. Comparing with the DOS of pure Al, the DOS of Al p and Mg s have sharp peaks at the equivalent energy. It illuminates that hybridizations exist between Al p and Mg s orbitals. The interesting hybridization effect implies the Al–Mg bonding has certain covalent character. The partly covalent Al–Mg bonding which is harder than the metallic Al–Al bonding in Al can effectively resist the elastic and plastic deformations. This is the reason that Al–5 wt%Mg has higher elastic moduli and ideal tensile strengths.

Besides, we have also computed the ideal tensile strength of Al–5 wt%Mg for the 108 atom supercell in the ⟨100⟩ direction. The value of ideal strength is 9.72 GPa and the critical strain is 0.263. These values are close to the results obtained for the 32 atom supercell (see Table II). It implies the 32 atom supercell is sufficient for modelling the mechanical properties of Al–5 wt%Mg.

3.3. Ideal compressive strength

When the strain is negative, the uniaxial tension turns into the uniaxial compression. The ideal compressive strengths of Al–5 wt%Mg still are not understood. Therefore, it is necessary to obtain the pressure limit of Al–5 wt%Mg through uniaxial compressive deformation of Al–5 wt%Mg using first-principles methods. The ideal compressive strengths have been calculated for a stress oriented in the ⟨100⟩, ⟨110⟩ and ⟨111⟩ directions. Table III gives the results of our calculated ideal compressive strengths and critical strains. For Al–5 wt%Mg, the ideal compressive strengths were identified in the ⟨100⟩ direction owing to the weakest peak compressive stresses as Table III showed. Thus, the pressure limit of Al–5 wt%Mg is 6.91 GPa with the corresponding strain of 0.114. It is noted that the ideal compressive strength of 38.96 GPa along ⟨110⟩ is evidently higher than 6.91 GPa and 10.26 GPa along ⟨100⟩ and ⟨111⟩. This also results from the strength of Al–Mg bonding which lies mainly through the ⟨110⟩ crystal direction. Figure 4 presents the stress–strain curves for Al–5 wt%Mg in ⟨100⟩, ⟨110⟩,

TABLE III

The ideal compressive strength and critical strain for Al–5 wt%Mg

Loading configuration	Ideal strength [GPa]	Critical strain
⟨100⟩ compressive	6.91	0.114
⟨110⟩ compressive	38.96	0.166
⟨111⟩ compressive	10.26	0.132

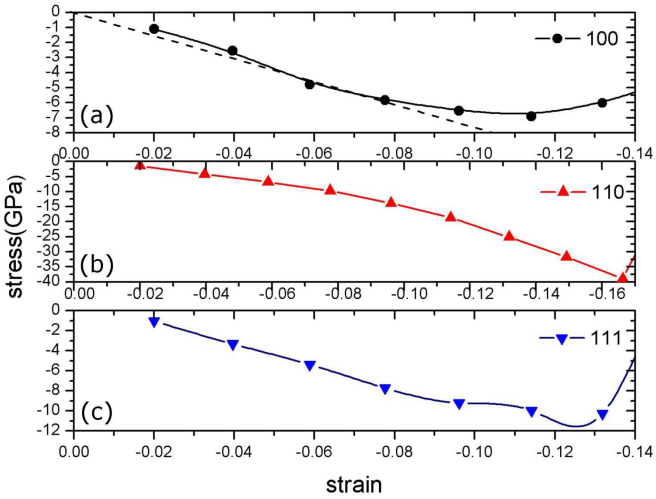

Fig. 4. The stress–strain relationships of Al–5 wt%Mg under compression loading.

and ⟨111⟩ compression. For the compressive deformation along the ⟨100⟩ direction, we can find a short region of a linear behavior near the origin. The fixed slope of the stress–strain curve indicates that the present deformation is an elastic deformation. The slope of the dotted straight line is 79.4 GPa, which is almost equal to our calculated Young's modulus of Al–5 wt%Mg (76.1 GPa).

In the end of this section, we give the ideal compressive strength of 6.85 GPa along ⟨100⟩ with the corresponding strain of 0.114 for the 108 atom supercell. We can see that these values are also close to the results obtained for the 32 atom supercell (see Table III). It further confirms the 32 atom supercell is sufficient for modelling the mechanical properties of Al–5 wt%Mg.

4. Conclusions

In summary, we have presented first-principles calculations of the structural, elastic, tensile, and compressive properties of Al–5 wt%Mg. The optimized lattice constant have been compared excellently with previous works. We first assess the accuracy of our computational approach on the mechanical properties by considering pure Al. Then the elastic constants, shear modulus, Young's modulus, Poisson's ratio and the brittle/ductile characteristics of Al–5 wt%Mg are successfully obtained. The calculated results demonstrate that Al–5 wt%Mg has larger shear modulus and Young's modulus in contrast with Al. It can be judged that Al–5 wt%Mg is a harder material, consistent with its exploitation in Al precipitate-hardening mechanisms. Finally, the stress–strain relations and ideal strengths under tension and compression loading have been determined. Results show that Al–5 wt%Mg is found to have higher tensile strengths than Al. The electronic structures indicate certain covalent character in Al–Mg bonding arises from the hybridizations between Al p and Mg s orbitals. The partly covalent Al–Mg bonding which is harder than the metallic Al–Al bonding in Al can effectively resist the elastic and plastic deformations.

Acknowledgments

The authors would like to thank PengFei Yin for helpful comments and discussions.

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