FIRST-PRINCIPLES STUDY ON THE MECHANICAL PROPERTIES OF Al_2ZnTM ALLOYS

by

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The mechanical properties of Al_2*ZnTM (TM = Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, and Cd) alloys have been studied using the first-principles calculation. By analyzing the mechanical stability, it was found that* Al_2*ZnPd,* Al_2*ZnAg, and* Al_2*ZnCd are mechanically unstable, and the rest all mechanical stable. Therefore, in this work only studies the mechanical properties of* Al_2*ZnTM (TM = Y, Zr, Nb, Mo, Tc, Ru, and Rh), including Young's modulus, lattice constants, super cell volume, atomic weight and density. We found the Young's modulus maximum is* Al_2*ZnMo, the value is 239.01 GPa, the* Al_2*ZnMo has maximum stiffness. The density of* Al_2*ZnRu its maximum value 6586.00 kg/m*^{3}*. In summary, studying the mechanical properties of* Al_2*ZnTM provides more options for optimal design and advanced application of* Al_2*ZnTM alloys.*

Keywords: *fist-principles, mechanical stability, Young's modulus, alloys, density*

Instructions

The Al-Zn series alloys have good mechanical properties such as high intensity, good ductility, and corrosion resistance [1, 2]. The Al-Zn series alloys are widely studied due to excellent mechanical performance, thermodynamic performance and corrosion resistance [3, 4]. In recent years, the theoretical research and experimental research of the Al-Zn series of alloys have achieved many results. The theoretical research of Al-Zn alloy is mainly based on the type of doping elements, the content of mixed elements, and the improvement of the structure of the alloy structure [5-7]. The experimental research on Al-Zn alloy is mainly based on the preparation process, the annealing process, and the solid solution process. First principles of research methods, nanoindentation experiments, SEM, XPS methods are powerful tools for studying Al-Zn alloy mechanical properties [8-11]. Adding rare earth, transition metal, and non-metals to Al-Zn alloys can improve their mechanical performance, thermodynamics and corrosion resistance. Doping elements, such as li, Si, Mg, Cu, Sn, Ni, Ce, Pt, and other rare earth, transition metal and non -metals. Its mechanical properties and corrosion resistance have obviously improved [12-17]. A large number of studies have shown that the diversification of alloy composition can significantly improve the Al-Zn alloy significantly improved Al-Zn alloy comprehensive performance [18-21].

In this work, based on first principles calculation, the mechanical properties of Al_2ZnTM (TM = Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd) alloy are studied.

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Computational methods

In this work, The first-principles calculation is used to study the properties of Al_2ZnTM (TM = Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd) through the density functional theory using a plane-wave pseudopotential method as implemented in the Cambridge sequential total energy package (CASTEP) code [20, 22, 23]. The generalized gradient approximation (GGA) within the Perdew, Burke, and Ernzerhof scheme is used to obtain the exchange-correlation potential. To ensure calculation precision, set up higher calculation accuracy, we employ the plane-wave energy cutoff of 600 eV, and the Brillouin-zone sampling mesh parameters for the k-point set of 6 × 6 × 6. The other parameters use the default settings of ultra-fine accuracy.

In this work, Al_3Zn compound were obtained by substituting one vertex Al atom with one Zn atom in a 1 × 1 × 1 Al_4 supercell models as shown in fig. 1(a). The supercell contain three Al atoms and one Zn atom, the supercells were used to study the mechanical properties of Al_3Zn. Al_2ZnTM compound were obtained by substituting one Al atom with one TM atom in a Al_3Zn supercell models as shown in fig. 1(b). The supercell contain two Al atoms, one Zn atom and one TM atom, the supercells were used to study the mechanical properties of Al_2ZnTM.

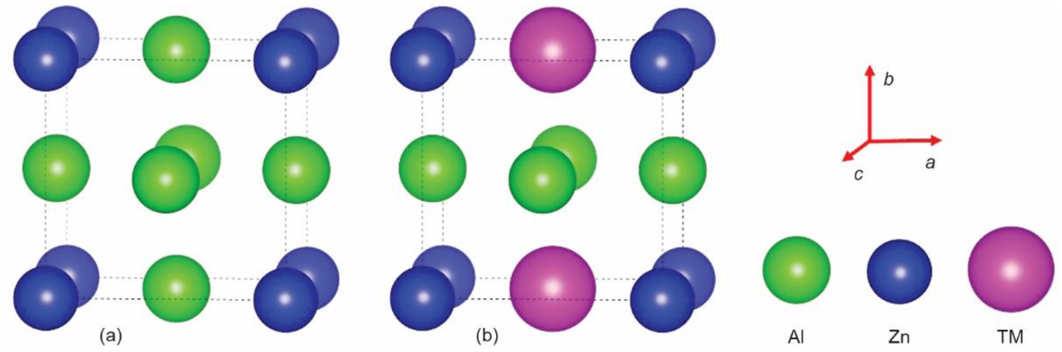

Figure 1. (a) The supercell models of Al_3Zn and (b) the supercell models of Al_2ZnTM

Results and discussion

Elastic constants and mechanical stability

Elastic constants of crystals provide a link between mechanical and dynamical behaviors. The elastic constants includes the elastic stiffness constants and the elastic flexibility constants. The elastic flexibility matrix S_{ij} and the elastic stiffness matrix C_{ij} are inverse matrices, that is $S_{ij} = C_{ij}^{-1}$, they for important information concerning the elastic response of a crystal to an external pressure. Elastic constants are important parameters to describe mechanical properties of solids. This elastic matrix has size 6 × 6 and it is symmetric. The higher the crystal symmetry, the fewer independent elastic stiffness constants there are. There are a maximum of 21 independent elastic stiffness constants. The elastic constants, C_{ij}, for orthorhombic Al_2ZnTM supercell predicated by GGA method. According to the elastic constants, it is found that Al_2ZnTM belongs to orthorhombic crystal. The mechanical stabilities of crystal structure under isotropic pressure can be determined by the criteria of independent elastic constants, C_{ij}. For an orthorhombic crystal, there independent components as shown in the following equation [24-26]:

$$\begin{gathered} C_{ii} > 0, \quad C_{11} + C_{22} - 2C_{12} > 0 \\ C_{11} + C_{33} - 2C_{13} > 0, \quad C_{22} + C_{33} - 2C_{23} > 0 \\ C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23}) > 0 \end{gathered} \tag{1}$$

According to the criteria, except for Al_2ZnPd, Al_2ZnAg, and Al_2ZnCd, all Al_2ZnTM is mechanically stable at ambient pressure. Therefore, the following will only study the mechanical properties of Al_2ZnTM (TM = Y, Zr, Nb, Mo, Tc, Ru, Rh).

Young's modulus

Young's modulus is one of the important mechanical properties of a materials. It is an important parameter that determines the deformation characteristics and stiffness characteristics of a material. The spatial distribution of Young's modulus can be expressed by the elastic flexibility coefficient S_{ij} of the material. The spatial distribution of the Young's modulus of orthorhombic crystals system can be expressed by [27]:

$$\frac{1}{E} = S_{11}l_1^4 + S_{22}l_2^4 + S_{33}l_3^4 + (2S_{12} + S_{66})l_1^2l_2^2 + (2S_{13} + S_{55})l_1^2l_3^2 + (2S_{23} + S_{44})l_2^2l_3^2 \tag{2}$$

where E is the Young's modulus, l_1, l_2 and l_3 are the directional cosine. Express E, l_1, l_2 and l_3 in rectangular coordinates, it can be written:

$$\begin{gathered} E = \sqrt{x^2 + y^2 + z^2}, \quad l_1 = \frac{x}{\sqrt{x^2 + y^2 + z^2}} \\ l_2 = \frac{y}{\sqrt{x^2 + y^2 + z^2}}, \quad l_3 = \frac{z}{\sqrt{x^2 + y^2 + z^2}} \end{gathered} \tag{3}$$

According to eq. (3), eq. (2) can be transformed into the eq. (4). According to eq. (4), the spatial distribution of the Young's modulus of Al_3Zn and Al_2ZnTM alloys is plotted, as shown in fig. 2:

$$\begin{aligned} (x^2 + y^2 + z^2)^{3/2} = {} & S_{11}x^4 + S_{22}y^4 + S_{33}z^4 + (2S_{12} + S_{66})x^2y^2 + \\ & +(2S_{13} + S_{55})x^2z^2 + (2S_{23} + S_{44})y^2z^2 \end{aligned} \tag{4}$$

The Young's modulus of Al_3Zn and Al_2ZnTM is shown in fig. 2. Young's modulus of Al_3Zn and Al_2ZnTM are exhibits anisotropy characteristics. The Young's modulus of Al_3Zn and Al_2ZnY are similar. The Young's modulus of Al_2ZnZr, Al_2ZnNb, Al_2ZnMo, Al_2ZnTc, Al_2ZnRu, and Al_2ZnRh are very different from that Al_3Zn. In particular, the Young's modulus of Al_2ZnMo, Al_2ZnTc, Al_2ZnRu, and Al_2ZnRh changes particularly significantly compared with the Young's modulus of Al_3Zn.

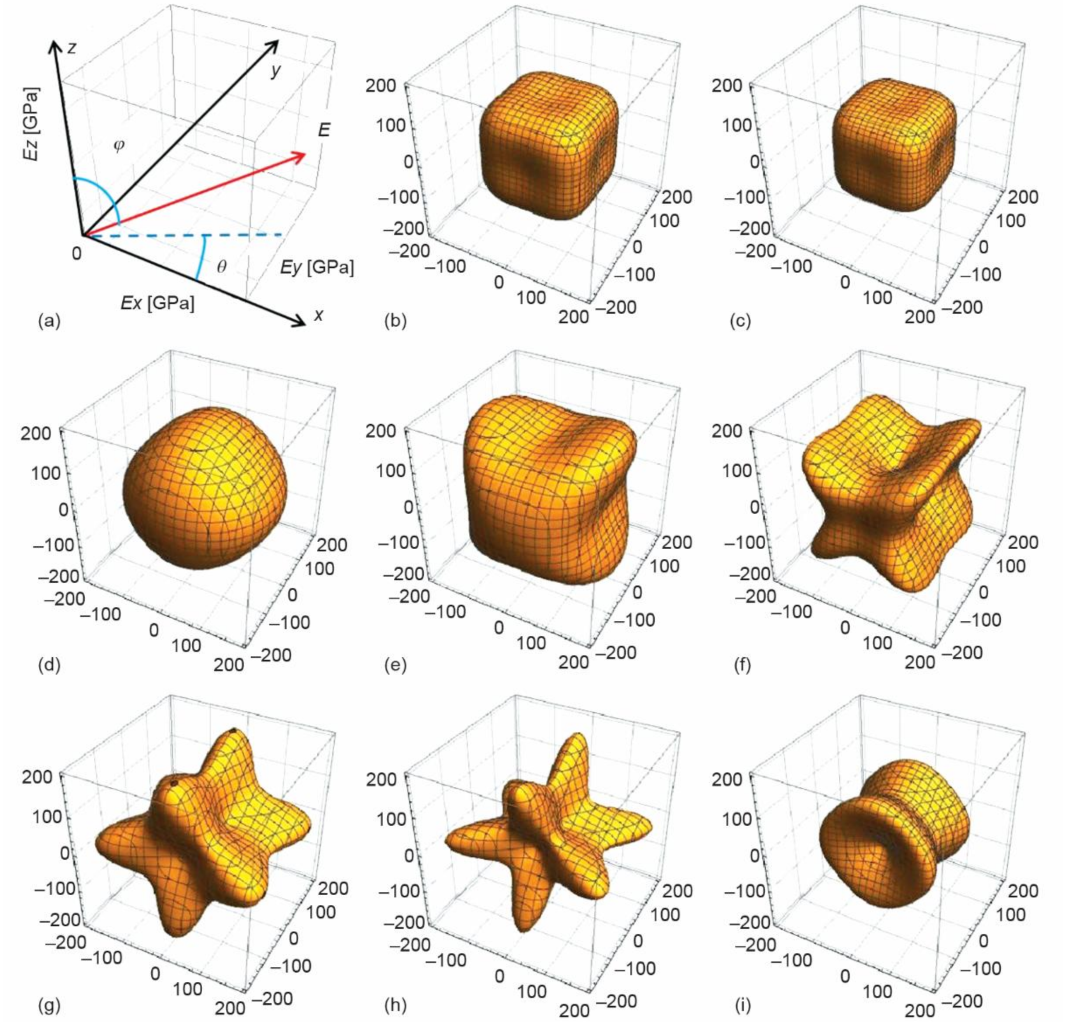

Figure 2. (a) The coordinate system, (b) the Young's modulus of Al_3Zn, (c) the Young's modulus of Al_2ZnY, (d) the Young's modulus of Al_2ZnZr, (e) the Young's modulus of Al_2ZnNb, (f) the Young's modulus of Al_2ZnMo, (g) the Young's modulus of Al_2ZnTc, (h) the Young's modulus of Al_2ZnRu, and (i) The Young's modulus of Al_2ZnRh

Since elements Y belong to the IIIB group elements and element Al belong to the IIIA group elements, because they have similar electronic shell structures, the Young's modulus of Al_3Zn and Al_2ZnY characteristics are also similar. Because the electronic shell structures of Mo, Tc, Ru and Rh are very different from Al, the Young's modulus characteristics of Al_2ZnMo, Al_2ZnTc, Al_2ZnRu, and Al_2ZnRh are also very different the Young's modulus characteristics of Al_3Zn. Because the electronic shell structure of Mo, Tc, Ru and Rh are complex, the Young's modulus spatial distribution of Al_2ZnMo, Al_2ZnTc, Al_2ZnRu, and Al_2ZnRh also exhibits a more complex shape.

The spatial distribution of Young's modulus of Al_3Zn and Al_2ZnTM exhibits anisotropic characteristics, while also being symmetric about the coordinate axis. This phenomenon is one of the important characteristics of single crystals, exhibiting both anisotropy and symmetry.

For this types of elastic anisotropy alloys material, researchers are more concerned about the maximum and minimum values of Young's modulus, as well as the corresponding directions. According to eq. (2), the maximum values, minimum values of Young's modulus of Al_3Zn and Al_2ZnTM and the corresponding directions are studied. The conclusions are shown in tab. 1. The direction is represented by θ and φ, and the direction of θ and φ is consistent with the direction in fig. 2(a).

Table 1. The maximum values, minimum values of Young's modulus and directions

Alloys	Maximum			Minimum		
	θ [°]	φ [°]	E [GPa]	θ [°]	φ [°]	E [GPa]
Al_3Zn	45.0	54.5	175.44	0.0	90.0	121.19
Al_2ZnY	43.5	54.0	157.54	0.0	90.0	110.60
Al_2ZnZr	40.5	90.0	184.71	0.0	45.0	167.3
Al_2ZnNb	0.0	45.0	237.98	0.0	0.0	139.08
Al_2ZnMo	50.5	57.5	239.01	0.0	90.0	52.22
Al_2ZnTc	90.0	38.0	245.85	0.0	45.0	70.01
Al_2ZnRu	36.0	90.0	234.84	0.0	45.0	45.97
Al_2ZnRh	90.0	36.5	170.87	900	90.0	54.54

The maximum values, minimum values of Young's modulus and directions are shown in tab. 1. The Young's modulus maximum is Al_2ZnMo, the value is 239.01 GPa, the direction of (θ, φ) is (50.5, 57.5). The Young's minimum is Al_2ZnRu, the value is 45.97 GPa, the direction of (θ, φ) is (0.0, 45.0).

The anisotropic properties of Young's modulus make the stiffness of the material exhibit anisotropy, the direction stiffness with the largest Young's modulus is also the largest, and the direction stiffness with the smallest Young's modulus is also the smallest. When applying single crystal materials, the loading direction can be reasonably selected according to the anisotropic characteristics of the stiffness, so that the mechanical properties can be optimized.

Lattice constants and volume

The lattice constants and super cell volume are the basic properties of matter. This paper studies the lattice constants and super cell volume of Al_3Zn and Al_2ZnTM. The resulting are presented in fig. 3. The dash line denotes the lattice constants and super cell volume of Al_3Zn.

The lattice constant a and lattice constant b of Al_2ZnNb and Al_2ZnRh are decrease, while the others Al_2ZnTM increase. The lattice constant b of Al_2ZnY and Al_2ZnZr are increase, while the others Al_2ZnTM decrease. The super cell volume of Al_2ZnY and Al_2ZnZr are increase, while the others Al_2ZnTM decrease.

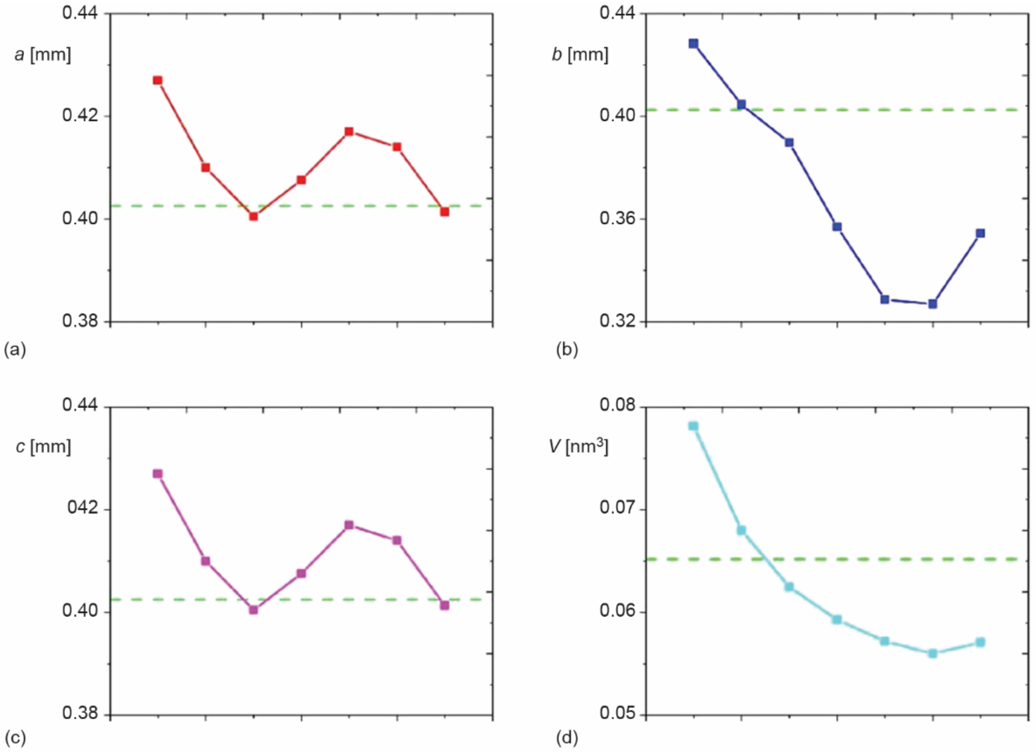

Figure 3. (a) The lattice *a* of Al_2ZnTM, (b) the lattice *b* of Al_2ZnTM, (c) the lattice *c* of Al_2ZnTM, and (d) the volume of Al_2ZnTM

Atomic weight and density

The atomic weight of the super cell and density are also basic properties of matter. This paper studies the atomic weight of the super cell and density of Al_3Zn and Al_2ZnTM. The resulting are presented in fig. 4. The dash line denotes the atomic weight of the super cell and density of Al_3Zn.

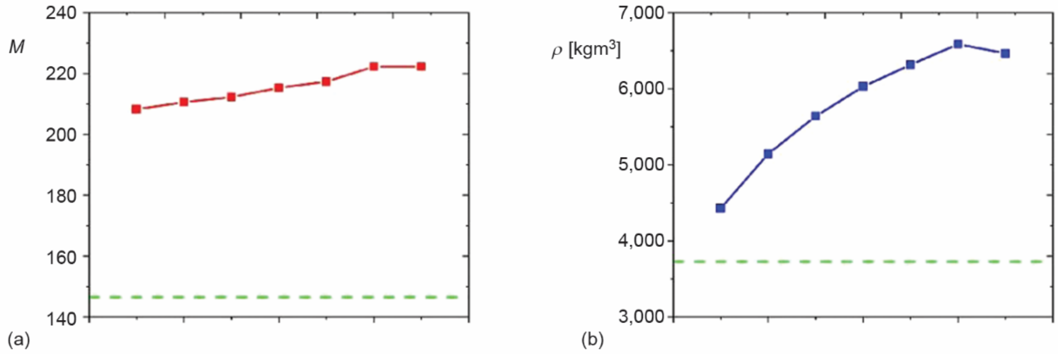

Figure 4. (a) The atomic weight *M* of Al_2ZnTM and (b) the density of Al_2ZnTM

Compared with Al_3Zn, the atomic weight M of super cell of Al_2ZnTM all increase. The atomic weight of Al_2ZnRu and Al_2ZnRh is the largest, with a value of 222.27. The atomic weight of $Al_2ZnY$is the smallest, with a value of 208.28. Compared with Al_3Zn, the density of Al_2ZnTM all increase. The density of Al_2ZnRu is the largest, with a value of 6586.00 kg/m^3. The density of Al_2ZnY is the smallest, with a value of 4428.37 kg/m^3.

Specific stiffness

Specific stiffness is an important indicator for measuring the lightweight properties of materials. Specific stiffness is defined:

$$\eta = \frac{E}{\rho} \tag{5}$$

The specific stiffness of of Al_3Zn and Al_2ZnTM are shown in tab. 2. The greater the specific stiffness value, the higher its application value. Compared with the Al_3Zn, the specific stiffness of Al_2ZnTM has decreased. The specific stiffness of Al_2ZnY, Al_2ZnZr, Al_2ZnNb, Al_2ZnMo, Al_2ZnTc, and Al_2ZnRu is not significantly reduce, and their specific stiffness values are greater than 0.035. The specific stiffness of Al_2ZnRh is obviously reduce, the specific stiffness value is only 0.0264.

Table 2. The specific stiffness of Al_3Zn and Al_2ZnTM

Alloys	Al_3Zn	Al_2ZnY	Al_2ZnZr	Al_2ZnNb	Al_2ZnMo	Al_2ZnTc	Al_2ZnRu	Al_2ZnRh
Specific stiffness	0.0471	0.0356	0.0359	0.0422	0.0396	0.0389	0.0356	0.0264

Conclusions

In this work, based on first-principles calculations, the mechanical properties of orthorhombic Al_2ZnTM (TM = Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd) crystals were studied. Analysis of mechanical stability revealed that Al_2ZnPd, Al_2ZnAg, and Al_2ZnCd are mechanically unstable, so subsequent investigations focused on Al_2ZnTM with TM = Y, Zr, Nb, Mo, Tc, Ru, and Rh.

Key findings include that Al_2ZnMo exhibits the maximum Young's modulus (239.01 GPa) and thus the highest stiffness. Al_2ZnRu has the maximum density (6586.00 kg/m^3). Additionally, the Young's modulus of these alloys shows anisotropic characteristics, and their lattice constants, supercell volumes, atomic weights, and specific stiffness values vary with the doped TM element, with Al_2ZnNb maintaining a relatively high specific stiffness (0.0422) close to that of Al_3Zn.

The mechanical properties of Al_2ZnTM alloys, particularly the high stiffness of Al_2ZnMo, the balanced lightweight and stiffness potential of Al_2ZnNb, and the controllable anisotropy of Young's modulus, indicate potential for engineering applications, including in micro-electro-mechanical systems [28-30] where high structural stability, lightweight properties, and directional mechanical performance are demanded. However, to determine specific application scenarios, further studies on additional properties such as electrical conductivity, thermal stability, microfabrication compatibility, and long-term reliability (*e.g.*, fatigue and corrosion resistance) are required, as these are not addressed in the present work.

Overall, this research provides a theoretical basis for understanding the mechanical properties of Al_2ZnTM alloys and lays a foundation for their potential application development.

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References

[1] Liu, L., *et al.*, Mechanical Property of Intermetallic Compounds in Zn-Al Solder Interconnects by Nanoindentation and First-Principles Calculations, *Intermetallics, 172* (2024), 108387
[2] Guo, K., *et al.*, Enhanced Combustion Performance of Al-Zn Alloys with Property Optimization Inspired by "Two-Way Tunneling" Strategy, *Surface and Coatings Technology*, *494* (2024), 131444
[3] Liu Y., *et al.*, Thermodynamic Re-Assessment of the Al-Li-Zn System, *Calphad, 87* (2024), 102752
[4] Wang, J., *et al.*, Study on the Microstructure and Corrosion Resistance of Hot-Dip Al-Zn-Si-xMg Coating, *Surface and Coatings Technology, 496* (2025), 131654
[5] Jeong, D. H., *et al.*, Microstructure and Mechanical Properties of High-Strength Al-Zn-Mg-Ni Alloys with Excellent Twin-Roll Castability, *Journal of Materials Research and Technology*, *33* (2024), Nov., pp. 5064-5074
[6] Li, C. M., *et al.*, First-Principles Calculations of Elastic and Thermodynamic Properties of the Four Main Intermetallic Phases in Al-Zn-Mg-Cu Alloys, *Computational Materials Science*, *93* (2014), Oct., pp. 210-220
[7] Liu, Z. Q., *et al.*, First-Principles Insights into Solute Partition among Various Nano-Phases in Al-Cu-Li-Mg Alloys, *Transactions of Nonferrous Metals Society of China*, *34* (2024), 6, pp. 1734-1744
[8] Du, B., *et al.*, Assessment of Thermal Conductivity for FCC Al-X (X=Zn, Mg) and Al-Zn-Mg Alloys: Experiments and Modeling, *Calphad, 87* (2024), 102763
[9] Chen, Y., *et al.*, Enhancing the Mechanical Properties of Mg-Zn-Al-Cu-Mn Alloy via $MgCO_3$ Inoculation Treatment: Experimental Studies and First-Principles Calculations, *Materials & Design*, *235* (2023), 112385
[10] Beyss, O., *et al.*, An In-Depth Investigation of the Native Oxide Formed on Al-Zn-Mg-Cu Alloys by XPS, XRR and ToF-SIMS, *Applied Surface Science*, *687* (2025), 162258
[11] Li, Z. L., *et al.*, Effect of Ce Content and Rolling Route on the Microstructure and Mechanical Properties of High-Zn Content Al-Zn-Ce Alloys, *Intermetallics*, *176* (2025), 108559
[12] Han, S. Z., *et al.*, Simultaneous Enhancement of Strength and Ductility in Al-Zn-Cu Casting Alloy with Trace Mg Addition Designed by First Principle Calculation, *Materials & Design, 244* (2024), 113140
[13] Yin, H., *et al.*, Investigation on Precipitate Behavior and Mechanical Properties of Al-Zn-Mg-Cu Alloys with Various Zn/Mg Ratios, *Journal of Materials Research and Technology*, *33* (2024), Nov., pp. 5769-5783
[14] Yang, M., *et al.*, Effect of Cu on Precipitation Hardening and Clustering Behavior of Al-Zn-Mg Alloys in the Early Stage of Aging, *Materials Characterization*, *219* (2025), 114632
[15] Wang, S., *et al.*, Study on Corrosion Behavior II of Hot-Dipped Zn-6Al-3Mg Alloy Coating: Surface Oxide Layer and Ternary Eutectic Corrosion, *Journal of Alloys and Compounds*, *1008* (2024), 176534
[16] Wang, G., *et al.*, Effects of Rare Earth Element Content on the Microstructural Properties and Corrosion Resistance of Al-Zn Alloy, *Materials Research Bulletin*, *184* (2025), 113227
[17] Yang, H., *et al.*, Effect of Homogenization Treatment on Microstructure and Properties of Novel Al-Mg-Zn-Sc-Zr Alloys with Different Mg/Zn Ratios, *Journal of Alloys and Compounds*, *1010* (2025), 177355
[18] Seo, N., *et al.*, Microstructural Evolution and Aging Behavior of Multicomponent Al-Sn-Zn-Mg-Li Alloy, *Journal of Alloys and Compounds*, *1011* (2025), 178381
[19] Zhang, Z., *et al.*, Design, Preparation, and Double-Mechanism Strengthening Effect Analysis of Sn-Zn-Al-Pt Solder Alloy with High Service Performance, *Materials Science and Engineering A, 923* (2025), 147755
[20] Zhang, C., *et al.*, Composition Optimization for Al-Zn-Mg-Cu Alloys Based on Thermodynamics and First-Principles Calculations, *Computational and Theoretical Chemistry, 1201* (2021), 113293

[21] Guo, C., *et al.*, Understanding the Strengthening Mechanism and Corrosion Behavior of Al-Mg-Zn(-Ag) Alloys Treated by Non-Linear Heating Ageing, *Journal of Alloys and Compounds, 1010* (2025), 177600

[22] Guo, Y., *et al.*, First-Principles Study on Stability, Electronic, Mechanical and Thermodynamic Properties of Al-Cu-RE Ternary Compounds, *Solid State Communications, 287* (2019), Jan., pp. 63-67

[23] Iwaoka, H., *et al.*, First-Principles Calculation of Elastic Properties of Cu-Zn Intermetallic Compounds for Improving the Stiffness of Aluminum Alloys, *Computational Materials Science*, *174* (2020), 109479

[24] Wu, Z., *et al.*, Crystal Structures and Elastic Properties of Superhard IrN_2 and IrN_3 from First Principles, *Physical Review B*, *76* (2007), 054115

[25] Mouhao, F., *et al.*, Necessary and Sufficient Elastic Stability Conditions in Various Crystal Systems, *Physical Review B*, *90* (2014), 224104

[26] Jiang, A. F., *et al.*, First-Principles Study on the Mechanical Properties of $Al_{1-x}TM_xP$, *Thermal Science, 28* (2024), 3A, pp. 2277-2285

[27] Li, H., *et al.*, First-Principle Calculations of Structural, Elastic and Thermodynamic Properties of Fe-B Compounds, *Intermetallics*, *46* (2014), Mar., pp. 211-221

[28] He, J.-H., *et al.*, Variational Approach to Micro-Electro-Mechanical Systems, *Facta Universitatis - Series Mechanical Engineering*, *23* (2025), 4, pp. 649-655

[29] He, C. H., *et al.*, A Modified Frequency Formulation for Nonlinear Mechanical Vibrations, *Facta Universitatis - Series Mechanical Engineering, 23* (2025), 2, pp. 197-210

[30] He, J.-H., *et al.*, Modeling and Numerical Analysis for MEMS Graphene Resonator, *Frontiers in Physics, 13* (2025), 1551969

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