

FIRST-PRINCIPLES STUDY ON THE MECHANICAL PROPERTIES OF Al_2CuRu ALLOYS UNDER STRAIN

by

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In this paper, the mechanical properties of Al_2CuRu were calculated by applying uniaxial strain in the y-direction. Research findings indicate that when the strain reaches -14% or 10% , the mechanical stability condition is not met. Consequently, the present study focused exclusively on the mechanical properties of Al_2CuRu within the strain range of -13% to 9% . The stress-strain curve of Al_2CuRu under uniaxial strain was analysed, revealing that strain applied in the y-direction resulted in significantly greater stress in the y-direction compared to the x- and z-directions. When the strain was between -4% and 2% , the stress-strain curve exhibited a satisfactory linear pattern. However, when the strain exceeds 2% or -4% , a slight non-linear phenomenon becomes evident. It was observed that Al_2CuRu exhibited elastic deformation without significant plastic deformation. It was also found that stretching can adjust the elastic modulus of Al_2CuRu , reduce its Vickers hardness, and increase its ductility. The elastic modulus has a large range of regulation. The adjustable range of bulk modulus and Young's modulus exceeds 160 GPa. The Al_2CuRu has a relatively large range of elastic deformation and is a typical plastic material. It is one of the alternative materials for the super elastic alloy family. It is therefore concluded that the mechanical properties of Al_2CuRu can be regulated by applying uniaxial strain, thus expanding the application range of Al_2CuRu materials.

Keywords: first-principles, mechanical stability, strain, elastic modulus, vickers hardness

Introduction

The advent of Al alloys into the realm of commercial applications can be traced back to the 1970's, with ongoing research in this field continuing to the present day. The primary objective of research in this field is to enhance the mechanical properties of Al alloys, with a view to producing alloys that exhibit high strength, high hardness, and high ductility. The evolution of Al alloys has progressed from the earliest dual alloys to the study of ternary and even multiple alloys [1-3]. The development of these alloys has transitioned from a single-component structure to a more complex, multi-component configuration. Common metal elements such as Fe, Cr, Ni, Ti, Cu, and Zn can be used to formulate Al alloys [4-8]. Research has demonstrated that the diversification of alloys can lead to substantial enhancement in the overall performance of materials.

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The Al-Cu-based alloy, formed by the addition of Cu to Al, has been shown to exhibit enhanced mechanical properties, including hardness, ductility, and strength [9-11]. The addition of other elements to Al-Cu alloys, such as rare earth and alkaline metals, has been shown to enhance Yang's modulus, shear modulus, and ductility [12-17]. A substantial body of research has demonstrated that the diversification of alloys can substantially enhance the overall properties of Al alloys, with the addition of elements such as Li, Mg, and rare earth metals being particularly effective [17-20].

In the author's previous research, Al_2CuRu was found to exhibit both good ductility and Vickers hardness. Consequently, the present study aims to extend these findings by conducting a more in-depth investigation into the mechanical properties of Al_2CuRu . The specific work is to apply y -directions strain to Al_2CuRu , study its ultimate strain, and investigate the regulatory effect of strain on its mechanical properties. In this work, based on first principles, the mechanical properties of Al_2CuRu alloy are studied.

Computational methods

In this study, the first-principles calculation is utilised to investigate the properties of Al_2CuRu through the density functional theory employing a plane-wave pseudopotential method as implemented in the Cambridge Sequential Total Energy Package (CASTEP) code [20-22]. The CASTEP code is a powerful tool for studying the mechanical, electrical, magnetic, and optical properties of materials. In recent years, more and more researchers have adopted CASTEP code to study the properties of materials and have developed many new materials with advanced properties. The generalized gradient approximation (GGA) within the Perdew, Burke, and Ernzerhof scheme is utilised to obtain the exchange-correlation potential. In order to ensure calculation precision, it is necessary to employ the plane-wave energy cutoff of 600 eV, and the Brillouin-zone sampling mesh parameters for the k -point set of $6 \times 6 \times 6$. The remaining parameters are set to their default ultra-fine accuracy settings.

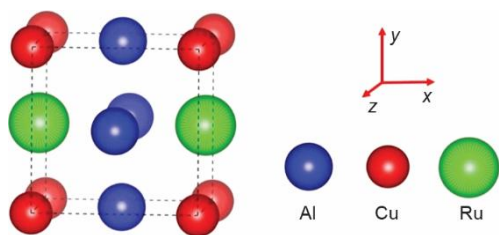


Figure 1. The supercell models of Al_2CuRu

In this work, Al_2CuRu compound were obtained by substituting two Al atom with one Cu atom and one Ru atom in a $1 \times 1 \times 1 \text{ Al}_4$ supercell models as shown in fig. 1. The supercell contain two Al atoms, one Cu atom and one Ru atom, the supercells were used to study the mechanical properties of Al_2CuRu .

For Al_2CuRu , the mechanical properties are calculated under strain conditions by applying uniaxial strain in the y -direction. The calculation process is divided into three steps:

- Set the corresponding uniaxial strain. Set the lattice constant in CASTEP, and the ideal single axis strain is applied here, that is, there is only response in the direction of y , no response in the x - and z -directions, and the crystal constant of the x - and z -direction remains constant.
- Geometric optimization of supercells. Only optimizing atomic positions without optimizing lattice constants. This geometric optimization method enables the atoms in the lattice to get the most stable position and maintain the corresponding strain.
- Calculate mechanical stability, elastic properties, including elastic stiffness constant and elastic modulus.

Results and discussion

Elastic constants and mechanical stability

Elastic constants of crystals provide a link between mechanical and dynamical behaviors. Also, 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_2CuRu supercell predicated by GGA method. According to the elastic constants, it is found that Al_2CuRu 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 [23, 24]:

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

Research has found that when the strain reaches -14% or 10% , the mechanical stability condition is not met. Therefore, the mechanical properties of Al_2CuRu were only studied when the strain was between -13% and 9% .

Stress-strain curve

The stress-strain, σ - ε , curve represents the variation law of stress with strain during solid deformation. According to Hooke's law, the stress-strain curer calculation formula for uniaxial strain can be derived. Among them, $\sigma_x(\sigma_y, \sigma_z)$ represents stress and Δy represents strain increment in the y -direction.

$$\begin{aligned} (\sigma_x)_i &= (\sigma_x)_{i-1} + C_{12}\Delta y \\ (\sigma_y)_i &= (\sigma_y)_{i-1} + C_{22}\Delta y \\ (\sigma_z)_i &= (\sigma_z)_{i-1} + C_{32}\Delta y \end{aligned} \quad (2)$$

According to eq. (2), the stress-strain curve of Al_2CuRu under uniaxial strain can be obtained, as shown in fig. 2. Applying strain in the y -direction results in a significantly greater stress in the y -directions than in the x -directions and z -directions. When Al_2CuRu is compressed, the σ_y - ε curve shows a good linear law, the σ_x - ε and σ_z - ε curves show a non-linear law. When Al_2CuRu is stretched, the σ_y - ε curve shows a non-linear law, the σ_x - ε and σ_z - ε curves show a good linear law. At all the deformation, Al_2CuRu is elastic deformation, and there is no obvious plastic deformation.

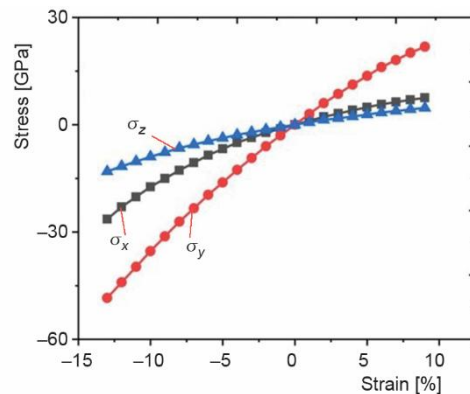


Figure 2. The stress-strain curve of Al_2CuRu in y -direction uniaxial strain

The elastic deformation range is 0 to –13% when compressed and 0 to 9% when stretched. Compression has a greater range of elastic deformation than tensile deformation. In general, Al₂CuRu has a relatively large range of elastic deformation and is a typical plastic material, it is one of the alternative materials for the super elastic alloy family.

Elastic modulus

The elastic modulus of polycrystalline is interconnected to the elastic constants of single crystals. Generally speaking, elastic properties of polycrystalline have greater practical significance than single crystal. Polycrystalline elastic properties are properties by bulk modulus, B , shear modulus, G , Young's modulus, E , and Poisson's ratio, μ . There are two models to evaluate the modulus: the Voigt method and Reuss method, which provide the upper and lower bounds of the polycrystalline elastic modulus, respectively. For different crystalline systems, the bulk modulus and shear modulus according to Voigt can be expressed as [25, 26]:

$$B_V = \frac{C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})}{9} \quad (3)$$

$$G_V = \frac{C_{11} + C_{22} + C_{33} - C_{12} - C_{13} - C_{23}}{15} + \frac{C_{44} + C_{55} + C_{66}}{5} \quad (4)$$

and by Reuss that:

$$B_R = \frac{1}{S_{11} + S_{22} + S_{33} + 2(S_{12} + S_{13} + S_{23})} \quad (5)$$

$$G_R = \frac{15}{4(S_{11} + S_{22} + S_{33}) + 3(S_{44} + S_{55} + S_{66}) - 4(S_{12} + S_{13} + S_{23})} \quad (6)$$

The bulk modulus and shear modulus can be obtained by the Voigt-Reuss-Hill method. The arithmetic average of Voigt and Reuss bounds is known as the Voigt-Reuss-Hill average, which is regarded as the best estimate for the theoretical value of polycrystalline elastic modulus:

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

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

The Young's modulus and Poisson's ratio can be computed based on the previous values by:

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

$$\mu = \frac{3B - 2G}{6B + 2G} \quad (10)$$

The B , G , E , and μ of Al_2CuRu are calculated according to eqs. (3)-(10). The calculation results are shown in fig. 3.

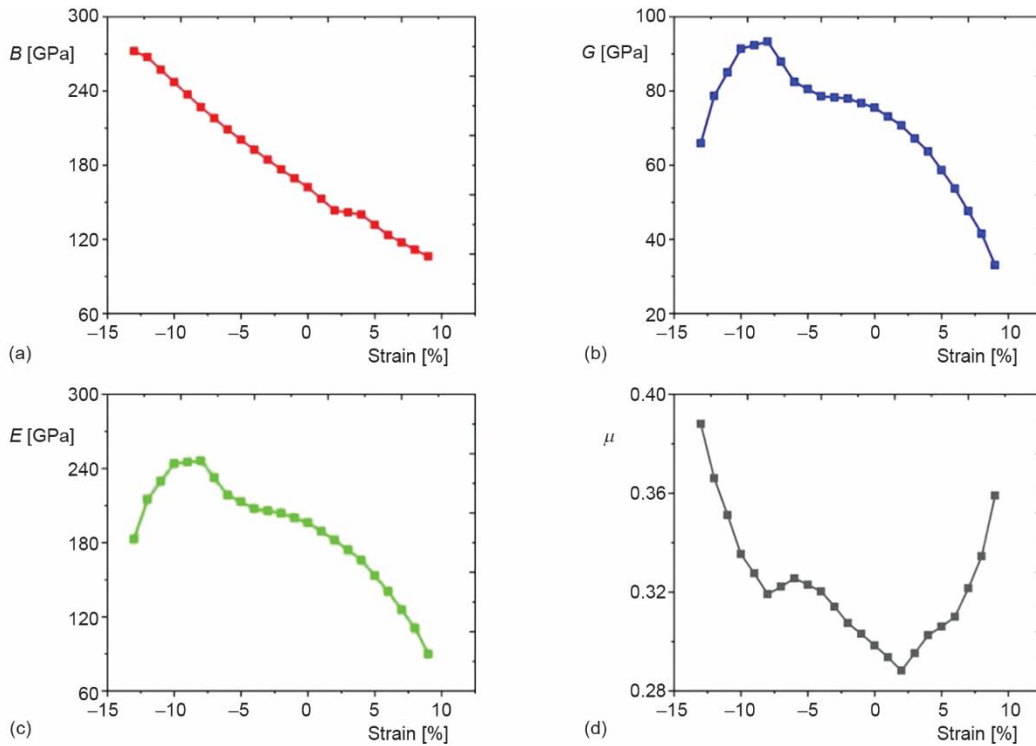


Figure 3. (a) The bulk modulus of Al_2CuRu , (b) the shear modulus of Al_2CuRu , (c) the Young's modulus of Al_2CuRu , and (d) the Poisson's ration of Al_2CuRu

The variation law of the bulk modulus, B , of Al_2CuRu with strain is shown in fig. 3(a). The overall trend is decreasing, with a maximum value is 272.30 GPa when the strain is -13% , with a minimum value is 106.19 GPa when then strain is 9% . The bulk modulus can be adjusted from 106.19 GPa to 272.30 GPa, with a control interval of 166.11 GPa.

The variation law of the shear modulus, G , of Al_2CuRu with strain is shown in fig. 3(b). It shows an approximately arched trend, with a maximum value is 93.33 GPa when the strain is -8% , with a minimum value is 33.05 GPa when then strain is 9% . The shear modulus can be adjusted from 33.05 GPa to 93.33 GPa, with a control interval of 63.28 GPa.

The variation law of the Young's modulus, E , of Al_2CuRu with strain is shown in fig. 3(c). It shows an approximately arched trend, with a maximum value is 246.24 GPa when the strain is -8% , with a minimum value is 89.82 GPa when then strain is 9% . The Young's modulus can be adjusted from 89.82 GPa to 246.24 GPa, with a control interval of 166.42 GPa.

The variation law of the Poisson's ratio, μ , of Al_2CuRu with strain is shown in fig. 3(d). With a maximum value is 0.39 when the strain is -13% , with a minimum value is 0.29 when then strain is 2% . The Poisson's ration can be adjusted from 0.29 to 0.39, with a control interval of 0.10.

According to the theory of mechanics of materials, the B , G , and μ satisfy by:

$$G = \frac{E}{2(1 + \mu)} \quad (11)$$

The B , G , and μ calculated in this work are verified by eq. (11), and it is found that they all meet the requirements of eq. (11). The theory of mechanics of materials also verifies that the calculation results in this paper are reliable.

Overall, the adjustable ranges of both the bulk modulus and the Young's modulus exceed 160 GPa, indicating that the adjustment range of the elastic modulus is relatively large.

Vickers hardness and ductility

The hardness of a material is the intrinsic resistance to deformation when a force is applied. Currently, a formal theoretical definition of hardness is still a challenge for material scientists. The hardness of a material is related to the elastic and plastic properties, there have been some semi-empirical model developed to predict the hardness of materials. Zhou *et al.* [27] proposed a model to predict the hardness of polycrystalline materials and bulk metallic glassed based on the Pugh's modulus ration ($k = G/B$) and the shear modulus:

$$H_V = 1.887k^{1.171}G^{0.591} \quad (12)$$

where H_V denotes the Vickers hardness.

The ratio of B/G can be used to estimate the ductility or brittleness of materials [28], since a high (low) value is associated with ductility (brittleness), and the critical value is about 1.75.

$$D = \frac{B}{G} \quad (13)$$

The H_V and B/G of Al_2CuRu are calculated according to eqs. (12) and (13). The calculation results are shown in fig. 4. The dashed line, fig. 4(b) represents the B/G is 1.75.

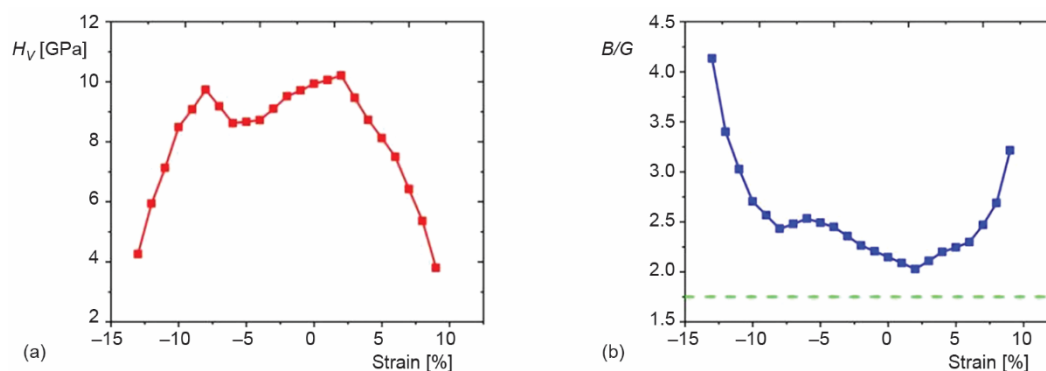


Figure 4. (a) The H_V of Al_2CuRu and (b) the B/G of Al_2CuRu

The variation law of the H_V of Al_2CuRu is shown in fig. 4(a). It shows an approximately arched trend, with a maximum value is 10.21 GPa when the strain is 2%, with a minimum value is 3.80 GPa when then strain is 9%. The strain is in the range of -10% to 4% , the Vickers hardness of Al_2CuRu changes are not significant. When the strain exceeds -10% or

exceeds 4%, the Vickers hardness of Al₂CuRu decreased dramatically. Therefore, excessive strain on Al₂CuRu is not conducive to improving the Vickers hardness of Al₂CuRu. The Vickers hardness can be adjusted from 3.80GPa to 10.21 GPa, with a control interval of 6.41 GPa.

The variation law of the *B/G* of Al₂CuRu is shown in fig. 4(b). With a maximum value is 4.13 when the strain is -13%, with a minimum value is 2.03 when then strain is 2%. Al₂CuRu are expressing better ductility, their *B/G* greater than 1.75. That is applying strain to the Al₂CuRu can significantly improve the ductility of the material. In particular, when the compressive strain exceeds -10%, the ductility of Al₂CuRu can greatly improved. The ductility can be adjusted from 20.3 to 4.13, with a control interval of 2.10.

Obviously, by adjusting the strain, it is not possible to obtain good Vickers hardness and ductility at the same time.

Elastic anisotropy

Several methods have been developed to estimate the elastic anisotropy of compound [27]. The bulk modulus anisotropy, *A_B*, shear modulus anisotropy, *A_G*, and for a crystal with orthorhombic symmetry can be determined:

$$A_B = \frac{B_V - B_R}{B_V + B_R}, \quad A_G = \frac{G_V - G_R}{G_V + G_R} \quad (14)$$

The *A_B* and *A_G* of Al₂CuRu are calculated according to eq. (14), the calculation results are shown in fig. 5. The zero value of anisotropic index (*A_B* or *A_G*) indicates that the crystal is iostropic. A high value of anisotropic index (*A_B* or *A_G*) means that the crystal structure has highly anisotropic elastic properties.

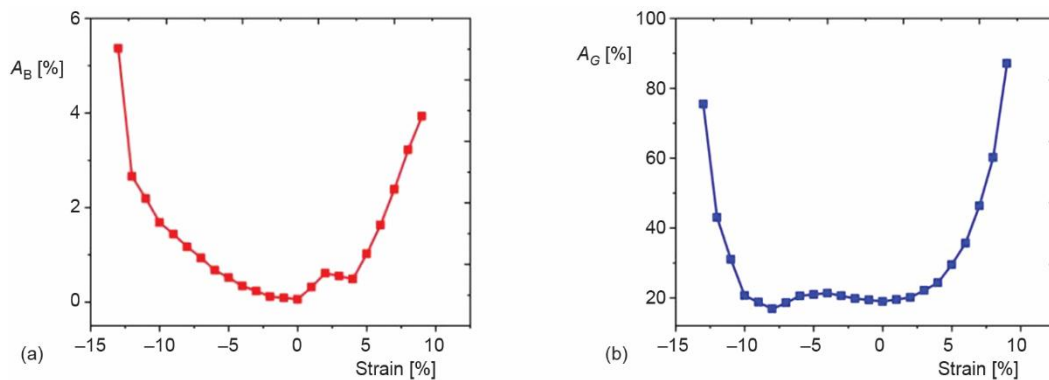


Figure 5. (a) The *A_B* of Al₂CuRu and (b) the *A_G* of Al₂CuRu

The bulk modulus anisotropy *A_B* of Al₂CuRu is shown in fig. 5(a). With a maximum value is 5.36% when the strain is -13%, with a minimum value is 0.06% when then No strain. In general, the bulk modulus anisotropy is very small, and the macroscopic is shows isotropic.

The shear modulus anisotropy *A_G* of Al₂CuRu is shown in fig. 5(b). With a maximum value is 87% when the strain 9%, with a minimum value is 18.98% when then No strain. The strain is in range of -10% to 4%, the shear modulus anisotropy does not change much.

When the strain exceeds -10 or exceeds 4% , the shear modulus anisotropy varies greatly and exhibits great anisotropy.

Conclusion

In this study, the mechanical properties of Al_2CuRu were calculated by applying uniaxial strain in the y -direction, and the mechanical stability of the material was analysed. It was found that when the strain reached -14% or 10% , the mechanical stability condition was not met. The findings of this study demonstrate that the mechanical properties of Al_2CuRu can be effectively regulated through the application of uniaxial strain in the y -direction, thereby expanding the application range of Al_2CuRu materials. The Al_2CuRu has a relatively large range of elastic deformation and is a typical plastic material. The elastic modulus has a large range of regulation. The adjustable range of bulk modulus and Young's modulus exceeds 160 GPa, which provides a new research: case for the exploration of metal material properties in the field of thermal science [29]. The research outcomes of this paper provide a theoretical foundation for the utilisation of Al_2CuRu alloy.

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