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Phase stability and mechanical properties of ternary transition elements X (X = Cu,Zn,Ag) in Al_3Hf intermetallic from first-principles calculations[☆]

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A R T I C L E I N F O

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A B S T R A C T

Site preference, phase stability and brittle *vs* ductile behaviors of ternary transition elements Cu, Zn and Ag in Al_3Hf intermetallic are investigated by using of first-principles calculations. It is found that it has a phase transition from $D0_{23}$ phase to $L1_2$ phase for Al_3Hf due to the strong Al site preference for Cu, Zn and Ag addition. It is shown that the role of activated antiphase boundaries on $\langle 110\rangle(001)$ plane is the key factor for the phase transition. Elasticity modulus show that ternary elements can effectively improve the ductility of Al_3Hf due to the phase transition. Finally, cleavage fracture model and slip fracture model were used to give a prediction of brittle to ductile transition mechanism based on Griffith fracture theory. The energetic results show that the improved ductility is due to the activated dislocation emission but suppressed crack propagation in materials.

1. Introduction

As a kind of high-temperature structural materials, Hafnium-aluminum (Hf-Al) intermetallic compound has attracted strong interests [1–3]. The excellent properties of Al_3Hf including good corrosion, relatively high melting point and high-temperature oxidation resistance of substrates, elevated temperature strength, relatively low density, and high melting point due to the abundant of Aluminum contains, which makes it widely used in the filed of advanced engineering materials [4,5]. However, the inherently brittle of Al_3Hf at room temperature which severely restricts its widespread applications. In view of this fatal defect, substantial experimental and theoretical efforts have been devoted to solve this problem. Earlier researches show that there are two noncubic phases in Al_3Hf, which are stable tetragonal $D0_{22}$-Al_3Hf or $D0_{23}$-Al_3Hf phases around 650 °C founded in experiments [6], while the higher structural symmetry $L1_2$ phase is thermally metastable. It means that the low structural symmetry under equilibrium lattice fails to provide a sufficient number of equivalent slip systems and presents poor ductility. Effective strategies show that the stabilization of high symmetry metastable $L1_2$ phase by ternary elements additions can provide more activated slip systems to satisfy von Mises criterion to improve its plastic [7]. One encouragement is that it can be transformed into the high symmetry cubic ordered $L1_2$ structure when Al atoms are partially replaced by transition metal elements and hopefully exhibiting good room-temperature ductility, according to previous research. So far, there are two methods to synthesize the $L1_2$ metastable phase: One is mechanical alloying (MA) method, which can obtain the single phase cubic $L1_2$ metastable phase, another one is the process of heat treating and the $L1_2$ cubic structure can be obtained from the supersaturate solid solution. For instance, the thermal stability of cubic ordered $L1_2$ structure can be obtained with the addition of 10 at.% Cu and 12.5 at.% Zn by mechanical alloying(MA) strategy [8]. Subsequently, similar researches also demonstrate that the cubic $L1_2$ phase is maintained with Zn addition [9]. Besides, the high aluminum content intermetallic compounds $D0_{23}$ and $L1_2$ phase Al_3Hf can directly formed by Hf ion implanted into Al matrix [10]. Recently, new identical researches show that the $L1_2$ phase can be stabilized with light element Li contains [11]. In general, the formation enthalpy can be used to characterize the phase stability of crystal. Moreover, the formation enthalpy of stable phase can be obtained from experimental methods, but it is difficult for the metastable phase. Nevertheless, theoretic calculation methods can elegantly solve this problem. The total energies and equilibrium cohesive properties have been investigated systematically by Ghosh and Asta [3] from first-principles calculation. The elastic properties in $L1_2$

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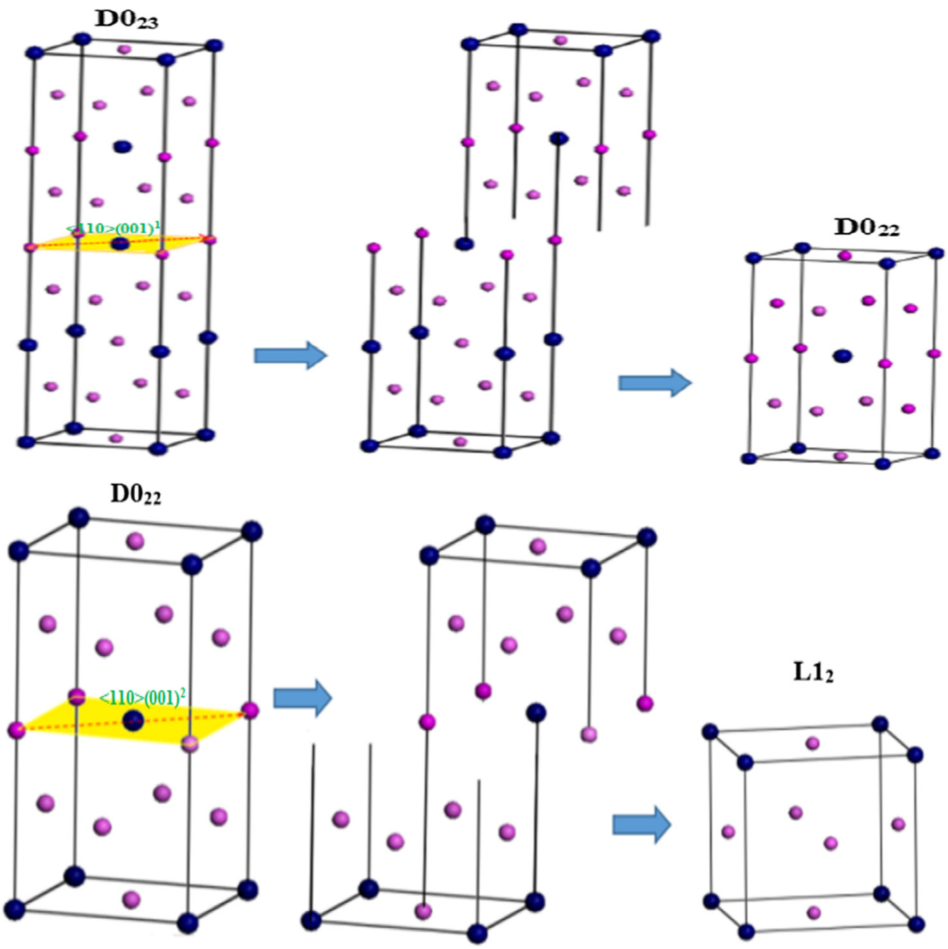

Fig. 1. The structure of $D0_{23}$, $D0_{22}$ and $L1_2$ phases Al_3Hf as well as phase transformations.

structure Al_3Hf and other $L1_2$ type intermetallic compounds have performed a systematic study by Tian's research team [12]. Unfortunately, accurate calculation of metastable $L1_2$-Al_3Hf is unclear. Furthermore, little reference to the mechanical properties and the phase transition mechanism as well as the brittle to ductile transformation mechanism are still lack of more deeper investigation due to the complexity of the brittle *vs* ductile mechanism. The structures of $D0_{23}$ and $L1_2$ phases are given in Fig. 1. We can see clearly that the higher symmetry cubic $L1_2$ phase is much closer to the lower symmetry tetragonal $D0_{23}$ phase. The low symmetry tetragonal $D0_{23}$ and $D0_{22}$ structures may be considered as super-structures of the simple cubic $L1_2$ cell. Furthermore, the cubic $L1_2$ phase can be supposed to be the transformation from the $D0_{23}$ phase with two two-step sliding processes: First step is from $D0_{23}$ phase to $D0_{22}$ phase by the $1/2\langle 110\rangle(001)^1$ antiphase shift in $(001)^1$ plane; Second step is from $D0_{22}$ phase to $L1_2$ phase also by the $1/2\langle 110\rangle(001)^2$ antiphase shift in $(001)^2$ plane (see Fig. 1). It implies that the ductility of Al_3Hf will be greatly improved once the transformation from the $D0_{23}$ phase to $L1_2$ phase occurs.

Based on the above analysis, our aim is to elucidate the intrinsic effects of ternary transition metal elements Cu, Zn and Ag on the ductile *vs* brittle behaviors of Al_3Hf from the following aspects: (a) Formation enthalpy is used to give a phenomenological predication of site preference. Stacking fault energy and charge density contour are given more microscopic views of transformation mechanism based on atomic and electronic scale from first-principles calculations; (b) Ductile *vs* brittle behaviors are distinguished phenomenologically by elastic modulus; (c) Deeper explanations of brittle to ductile transformation are given from the competitive mechanism between crack propagation and dislocation emission based on Griffith fracture theory.

2. Methods and computational details

In present work, first principles calculations were performed using the Vienna *ab initio* simulation package (VASP) code which has been described elsewhere [13,14]. VASP is a plane-wave code by using the iterative approach to achieve the structural optimization of the ground state. This approach needs to seek appropriate potentials. Meanwhile, the ultra-soft pseudo-potentials (USPP) can meet the demand of a modest cutoff for the plane-wave basis of transition metals. The exchange correlation energy was performed within the generalized gradient approximation (GGA) within PAW pseudo-potentials proposed by Perdew, Burke and Ernzerhof (PBE) [15] in all of our calculations. Valence electrons for Hf-$5s^25p^65d^26s^2$ and Al-$3s^23p^1$ including 5s semicore state as valence to tread this 5d transition metal element. Meanwhile, Monkhorst-Pack special k-point scheme was used to treat the Brillouin-zone integration [16]. The total energy is converged to less than 10^{-5} eV/atom and the Hellman-Feynman forces are converged toless than 0.01 eV/Å to ensure the accuracy of our calculations. After convergence tests, the cutoff energy for plane wave expansions was set as 450 eV. The k points separation in the Brillouin zone of the reciprocal space were 15 × 15 × 15, 15 × 15 × 7 and 15 × 15 × 5 for $L1_2$-Al_3Hf, $D0_{22}$-Al_3Hf and $D0_{23}$-Al_3Hf, respectively. The stacking fault energy as a function of the slip displacement u with the additional energy per unit area by shifting the upper half super cell relative to its lower as well as the cleavage energies as a function of the separation distance x between the neighboring cleavage planes were determined. A vacuum region of 12 Å was used to separate the parallel faults. Spin polarization was considered in all of our calculations to treat these transition elements.

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