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Strengthening effects of alloying elements W and Re on Ni_3Al: A first-principles study

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ABSTRACT

The structural stabilities, mechanical and thermodynamic properties of pure and alloyed Ni_3Al systems have been investigated systematically, based on density functional theory and Debye-Grüneisen model. Close attentions are paid to alloying elements W and Re by studying the strengthening effects of single-alloying element W, Re, Mo, Ta, Ru and co-alloying elements WRe, WMo, ReMo, WTa, ReTa, WRu, ReRu, which substitute the Al site and the nearest neighboring Al-Al sites, respectively. The calculated formation energies and elastic constants show that all the alloyed Ni_3Al are thermodynamically and mechanically stable. It is found that alloying elements W has similar effects on the mechanical and thermodynamic properties of Ni_3Al to those of Re, which suggests a possibility of replacing Re with W in Ni-based single crystal superalloys. In addition, co-alloyings with different elements have no distinct synergistic enhancement but simple combined effect on the mechanical properties of Ni_3Al. The enhanced chemical bondings between the alloying atoms W/Re and the neighboring host atoms Ni are considered to be the main strengthening mechanisms in W/Re alloyed Ni_3Al systems.

1. Introduction

Ni-based single crystal (SC) superalloys are widely used in most advanced gas-turbine systems and aero engines, owing to their outstanding mechanical properties and oxidation resistances at high temperature. The excellent comprehensive performances in the new generation of Ni-based superalloys benefit from the microstructure with high volume fraction of γ'-Ni_3Al (ordered $L1_2$) precipitates coherently embedding in γ-Ni matrix (disordered fcc (face-centered cubic)) [1,2], as well as many kinds of alloying elements (e.g. Mo, W, Re, Ta, Ru, Cr) [3]. A distinctive feature of the development of SC superalloys is the increasing concentration of Re, which has been proved to be a crucial element for the striking enhancement of mechanical properties. Unfortunately, the excessive addition of Re will lead to the precipitation of detrimental topologically close-packed phases (TCP), and hence the element Ru is added to suppress the formation of TCP. Since Re and Ru elements are scarce and expensive, the costs of SC superalloys with these elements increase sharply. Accordingly, alloy design aiming at reducing the additions of Re and Ru with minimal loss in service performance has become research focus, due to the urgent development of low-cost SC superalloys.

Recently, it has been reported that Mo and Re can strongly promote the precipitation of TCP phases, but W has no obvious effect on it [4–6]. This research inspires us to think whether the element Re can be partially replaced by W without degrading the mechanical and thermodynamic properties of SC superalloys. Previously, some single-alloying elements (e.g. Ta, Mo, W, Cr, Re, Ru, Co, and Ir) and co-alloying elements (Mo-Ta, Mo-Re, Mo-Cr) have been studied to evaluate their strengthening effects on SC superalloys by first-principles calculations respectively [7,8]. However, the results in the single-alloying of W and Re only provided limited evidence for the possibility of replacing Re with W in SC superalloys. Consequently, further comparison in the strengthening effects of W and Re in SC superalloys should be conducted systematically both in single- and co-alloying cases. As is known, the element W is roughly equally distributed in γ and γ' phases in most of superalloys [9], while the partitioning behavior of Re between γ and γ' is complex and varied with the composition of the SC superalloys. Recently, by atom-probe tomography (APT), some γ phase formation elements such as Mo and Re have been found in γ' precipitates

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as well and there is no sharp changing concentration profiles across the γ/γ' phase interface [10,11]. In addition, it has been reported that Re are enriched in the γ' matrix phase in some ternary and quaternary alloys [9]. More importantly, the excellent high temperature strength and creep resistance of SC superalloys rely primarily on the strengthening of γ' phases [12]. Therefore, it is essential to study the strengthening effects of W and Re in γ' phase in SC superalloys.

However, it is difficult to investigate the issue above on atomic scale by experimental methods, especially in terms of accuracy and costs. Whereas, first-principles approaches based on electronic density functional theory (DFT) have been proved to be powerful and reliable in predicting the properties of various alloying systems [13–15]. Therefore, in the present work, we perform a thorough investigation on the Ni_3Al systems single-alloyed with W, Re, Mo, Ru, Ta in two different concentrations, and co-alloyed with WRe, WMo, ReMo, WTa, ReTa, WRu, ReRu by means of DFT calculations. The elastic constants and moduli of these systems are calculated to evaluate the effects of these alloying elements on the mechanical properties of Ni_3Al, and the strengthening effects of W and Re co-alloyed with another alloying element are mainly compared at 0 K and finite temperatures. Moreover, the thermodynamic properties of different alloyed Ni_3Al systems are also calculated and compared to discuss the possibility of replacing Re with W in SC superalloys further. Finally, the charge transfer and chemical bonding between the alloying atoms and their nearest-neighboring atoms are analyzed to uncover the strengthening mechanism underlying.

2. Method and computational model

All the elastic stiffness constants of several Ni_3Al systems are calculated by using Vienna Ab initio Simulation Package (VASP) based on the electronic density functional theory (DFT) [16,17]. The Perdew, Burke, Ernzerhof exchange-correlation functional within generalized gradient approximations (GGA-PBE) is adopted for parameterization [18,19]. The projector augmented wave (PAW) pseudopotentials are used to take the core electrons into account [20]. After effective test calculations, the value of 500 eV is considered as the suitable cutoff energy for plane wave basis set, and a $5 \times 5 \times 5$ of Monkhorst-Pack k-points grids is adopted for Brillouin Zone sampling [21]. The convergence conditions of the electronic and ionic step in the self-consistent calculations are chosen to be 10^{-6} eV and 0.001 eV/Å based on our calculation model. Moreover, the contour maps of Differential Charge Densities (DCD) and Partial Density of States (PDOS) are calculated and analyzed [22]. And we use the quasi-harmonic Debye-Grüneisen model performed in the GIBBS2 code to obtain the thermodynamic parameters [23,24]. All the results in this work are obtained based on the spin-polarized calculations.

The basic model of our calculations is a periodic supercell composed of $2 \times 2 \times 2$ conventional cubic cells of γ'-Ni_3Al and contains 24 Ni and 8 Al atoms, which is chosen according to the alloying concentration and has proved to be effective to analyze the strengthening effect of alloying elements in SC superalloys [8,25]. Two alloying concentrations are considered in the present work. The configurations of the Ni_3Al supercells alloyed with single and double alloying atoms are shown in Fig. 1, which have the alloying concentration of 3.125 at.% and 6.25 at.% respectively. The single-alloying atom M (M: Re, W, Mo, Ta, Ru) substitutes the Al site and the atom pairs MN (MN: ReRe, WW, MoMo, TaTa, RuRu, WRe, WMo, ReMo, WTa, ReTa, WRu, ReRu) are placed in the nearest-neighboring Al-Al sites of Ni_3Al supercell in our calculations, according to the previous results obtained in alloyed γ'-Ni_3Al [7,8,12,26].

3. Results and discussion

3.1. Lattice parameters and thermodynamic stability

The calculated equilibrium lattice constants (a) of pure and alloyed Ni_3Al systems are shown in Table 1. The lattice constant of pure Ni_3Al (3.556 Å) agrees well with the experimental value [27], and all the alloying elements increase the lattice constant of Ni_3Al apparently.

In order to investigate the stabilities of the alloyed Ni_3Al systems, the formation energies E_{form} per unit cell have been calculated according to the following equation:

$$E_{form} = \left[E_{total}^{Ni_{24}Al_{8-m-n}M_mN_n} - 24E_{bulk}^{Ni} - (8-m-n)E_{bulk}^{Al} - mE_{bulk}^{M} - nE_{bulk}^{N}\right]/8 \quad (1)$$

where $E_{total}^{Ni_{24}Al_{8-m-n}M_mN_n}$ $(m, n \in N; m+n \leqslant 2)$ is the total energy of the alloyed Ni_3Al supercell shown in Fig. 1, and M, N represent the alloying atoms of the same or different type of elements. E_{bulk}^{Ni}, E_{bulk}^{Al}, E_{bulk}^{M}, E_{bulk}^{N} represent the ground state energies of the alloying atoms of Ni, Al, M and N in bulk respectively. The calculation results in formation energy are listed in Table 1. The formation energies are all negative for the alloyed Ni_3Al systems, which indicates the substitution reactions of these alloying elements are energetically favorable. Additionally, the alloying element Ta presents relatively stronger stabilizing effect with lowest formation energies in both single- and co-alloying cases. This result is consistent with the fact that Ta is a strong γ' formation element in Ni-based superalloys [9].

3.2. Elastic properties

Superalloys are applied in the extremely harsh environment, which puts forward very high demands on their mechanical prop-

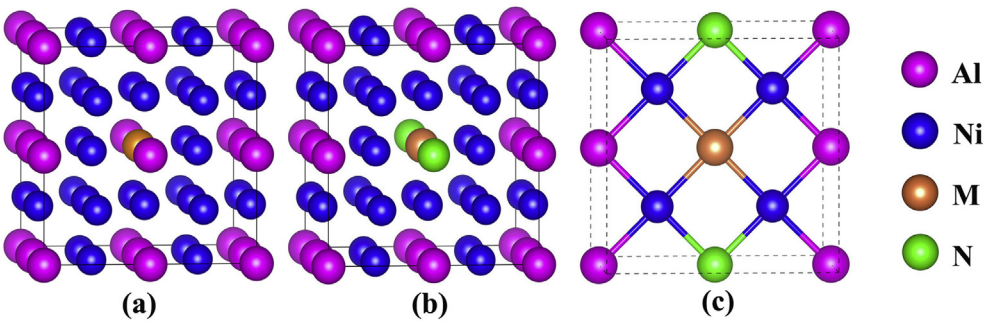

Fig. 1. The supercell of the alloyed systems (a) Ni_3Al-M (M: Re, W, Mo, Ta, Ru), (b) Ni_3Al-MN (MN: ReRe, WW, MoMo, TaTa, RuRu, WRe, WMo, ReMo, WTa, ReTa, WRu, ReRu), respectively. (c) The (0 1 0) atomic layer of the alloying configuration.