First-Principles Study of the Effects of Re and Ru Doping Content on the Stability of Ni-Al Binary Model Nickel-Based Single-Crystal Superalloys: Postprint

Authors: Zhifei Peng

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Abstract

First-principles calculations were employed to investigate the effects of doping element (Re, Ru) content on the stability and site preference in Ni-Al binary model single-crystal superalloys. The results indicate that with increasing Re and Ru content, the total energy of the system gradually decreases, demonstrating enhanced system stability. Concurrently, the system with Ru substituting Ni exhibits the lowest stability, whereas the system with Re substituting Al shows the highest stability; both Re and Ru demonstrate a preference for substituting Al, consistent with previous experimental findings. Furthermore, when the Re and Ru content is approximately 1.4% substituting Al, the substitution formation energy reaches its minimum compared to other Re and Ru concentrations. Additionally, two distinct stacking fault modes were obtained by removing a layer of atoms from the Ni-Al binary model. Investigations of these two stacking fault modes reveal that substituting Al with Re and Ru can improve system stability, with Re-containing systems being more stable and exhibiting lower substitution formation energies than Ru-substituted Al systems. However, for different stacking fault modes, the optimal Re and Ru contents required to achieve maximum system stability and minimum substitution formation and stacking fault energies differ. While substituting Al with Re yields stacking fault systems with superior stability, the Re content in the most stable system depends on the selected stacking fault mode.

Full Text

Abstract

Using first-principles calculations, we investigated the influence of doping element Y3 and Y2 content on the stability and site preference of a γ/γ' binary

model single-crystal superalloy. The results show that with increasing Y3 and Y2 element content, the total energy of the system gradually decreases, indicating that the stability of the system is improved. The system with Y2 replacing γ exhibited the lowest stability, while the system with Y3 replacing γ' showed the best stability. Both Y3 and Y2 preferentially substitute for γ', which is consistent with previous experimental results. Additionally, when the content proportion of Y3 and Y2 elements is approximately 1.4% replacing γ', the substitution formation energy is the lowest compared to other Y3 and Y2 contents. By removing one layer of atoms from the γ/γ' binary model, we obtained several different stacking fault modes. Studies on these stacking fault modes show that replacing γ' with Y3 and Y2 can improve system stability, and the Y3-containing system is more stable, with substitution formation energy also lower than that of Y2 replacing γ'. However, for different stacking fault modes, when using Y3 and Y2 to replace γ' at optimal system stability with lowest substitution formation energy and stacking fault energy, the required Y3 and Y2 contents differ. Using Y3 to replace γ', the stacking fault system has better stability, but the Y3 content in the most stable system depends on the selected stacking fault mode.

Keywords: γ/γ' binary model; first-principles calculations; Y3 and Y2 elements; stability; stacking fault mode

Introduction

Previous studies on the effects of doping elements on site preference and stacking fault energy in Ni-based single-crystal superalloys have focused on analyzing how substituting single atoms affects alloy stability. However, experimental studies of doping elements require not only strict experimental conditions and high material costs, but also face difficulties in precisely controlling the content of a series of doping elements. Compared with experimental methods, theoretical simulation offers advantages of low cost, high speed, and high efficiency, and can effectively investigate the physical mechanisms behind refractory element doping behavior at a more microscopic scale.

The influence of varying Y3 and Y2 content on the stability of Ni-based single-crystal superalloys remains largely speculative, lacking quantitative computational analysis. It remains unclear how much Y3 and Y2 doping is needed to achieve optimal stability and mechanical properties. This study establishes a γ/γ' binary model Ni-based single-crystal superalloy and two different stacking fault modes based on this model. Using first-principles calculations, we computed the energy variation trends of the γ/γ' binary model single-crystal superalloy when different numbers of Y3 and Y2 atoms replace existing atoms, to investigate how different Y3 and Y2 contents affect the stability, site preference, and stacking fault modes of Ni-based single-crystal superalloys.

Methodology

Model Construction

As shown in Figure A, investigating the Y3 and Y2 element content when the γ/γ' binary model Ni-based single-crystal superalloy has optimal stability. Computational model and formulas. The γ/γ' binary model Ni-based single-crystal superalloy consists of 100 atoms, including the γ phase Ni and the γ' phase Ni_3Al, where the lattice constants of γ and γ' are 3.52 Å and 3.57 Å respectively, obtained through self-consistent calculation of the system. The data is similar to results in literature. The upper layer of this model is the γ' phase Ni_3Al, the lower layer is the γ phase Ni, each layer consists of 50 atoms, which are obtained by unit cell expansion of Ni_3Al with $L1_2$ structure and Ni with FCC structure. A vacuum layer is added to the upper and lower layers to offset the periodic influence of the model in the Z-axis direction, as shown in Figure 1. Note: blue atoms are Al, gray atoms are Ni. Figure 1: γ/γ' binary model Ni-based single-crystal superalloy.

The total energy calculation of the model is based on density functional theory. The calculation software uses VASP. Under the generalized gradient approximation (GGA), the Perdew-Burke-Ernzerhof (PBE) exchange-correlation potential and projector augmented wave method (PAW) are selected for studying atom and electron optimization. In the calculations, the plane wave cutoff energy is selected as 400 eV, the electron self-consistent iteration convergence accuracy is set to 10^{-5} eV, atoms are relaxed until the Hellmann-Feynman force is less than 0.01 eV/Å. The k-points in the Brillouin zone are automatically generated using Monkhorst-Pack parameters, in self-consistent calculations, the value is $9 \times 9 \times 1$.

Note: (a), (b) indicate the number of Y3 or Y2 atoms replacing Ni atoms ranges from 1 to 4.

[Figure 1: see original paper] Schematic diagram of Y3 or Y2 replacing Ni atoms in the γ/γ' binary model

Note: (a), (b) indicate the number of Y3 or Y2 atoms replacing Al atoms ranges from 1 to 4.

[Figure 2: see original paper] Schematic diagram of Y3 or Y2 replacing Al atoms in the γ/γ' binary model

Stacking Fault Mode Construction

Based on the γ/γ' binary model, two different stacking fault modes were constructed by removing one layer of atoms while keeping the total number of atoms constant.

Energy Calculation Formulas

To investigate the effect of doping on single-crystal superalloy stability, Ni and Al in the γ' phase of the model were replaced with different numbers of Y3 or Y2 atoms to obtain models with varying dopant content. Additionally, to analyze the site preference and system stability at different doping contents, we calculated the total system energy and substitution formation energy. The substitution formation energy, denoted as E_{form}, is defined as follows: where C represents the doping element (Y3, Y2), M represents the element being replaced (Ni, Al), n represents the number of atoms being replaced, E_{tot} represents the total energy of the system after replacing n doping atoms, μ_M represents the chemical potential of a single replaced atom, μ_{Ni} is taken from FCC Ni, $\mu_{Al} = E_{Ni_3Al} - 3\mu_{Ni}$, E_{ref} represents the total energy of the system before refractory element replacement, μ_C represents the chemical potential of a single doping atom, taken from HCP Y3 and Y2.

Figure 3 Relationship between Y3 and Y2 element content and total system energy. As can be seen from Figure 3, the total energy of the system decreases with increasing doping element content, which means that as the content of Y3 and Y2 elements increases, the stability of the system gradually improves. In addition, the system with Y3 replacing Al has the lowest total energy, which indicates that this system has the best stability, while the system with Y2 replacing Ni has the highest total energy, therefore this system has the worst stability.

Based on the analysis of substitution formation energy, Y3 and Y2 elements preferentially substitute for Al atomic positions. Therefore, stacking fault modes only consider cases where dopant elements Y3 and Y2 replace Al.

Results

Stability Study of Stacking Fault Mode Q

Stacking fault mode Q was obtained by removing one layer of Ni atoms along the (111) plane direction in the γ/γ' binary model, as shown in [Figure 3: see original paper] (a). [Figure 4: see original paper], [Figure 5: see original paper], and [Figure 6: see original paper] display the trends of total energy, substitution formation energy, and stacking fault energy of mode Q as functions of Y3 and Y2 element content.

[Figure 4: see original paper] Relationship between Y3 and Y2 element content and total energy of stacking fault mode Q

As shown in [Figure 4: see original paper], the total energy variation trend is similar to that of the γ/γ' binary model. With increasing dopant content, the system total energy gradually decreases, indicating that system stability improves with increasing Y3 and Y2 content. The Y3-containing system consistently shows better stability than the Y2-containing system.

[Figure 5: see original paper] Relationship between Y3 and Y2 element content and substitution formation energy of stacking fault mode Q

[Figure 5: see original paper] shows the variation of substitution formation energy for stacking fault mode Q. When dopant content ranges from 0 to 1.4%, the substitution formation energy remains essentially stable. When Y3 or Y2 content exceeds this, consistent with research conclusions. Additionally, if Y3 content continues to increase, the stacking fault energy of the Y3-containing system basically does not change. When Y2 is 1.4%, the system substitution formation energy rapidly decreases. When Y3 content is approximately 2.1%, the substitution formation energy for Y3 replacing Al reaches its minimum. When Y2 content is approximately 2.8%, the substitution formation energy of the Y2-replacing-Al system is the lowest. Combined with analysis of total energy and substitution formation energy, it can be concluded that when Y3 content is approximately 1.4% and Y2 content is approximately 2.8%, each system readily undergoes doping phenomena. If Y3+Y2 content exceeds these values, doping behavior gradually becomes more difficult.

[Figure 6: see original paper] Relationship between Y3 and Y2 element content and stacking fault energy of stacking fault mode Q

[Figure 6: see original paper] reveals that when dopant content is below 1.4%, increasing dopant content can slightly increase the system stacking fault energy, which can be validated from previous research results. For Y3-containing systems, when Y3 content exceeds 2.1%, the system stacking fault energy decreases. While for Y2-containing systems, when Y2 content is greater than 2.8%, the stacking fault energy decreases. This indicates that when dopant Y2 content reaches a certain value, it can reduce the system stacking fault energy.

Stability Study of Stacking Fault Mode S

Stacking fault mode S was obtained by removing one layer of Ni atoms along the (111) plane direction in the γ/γ' binary model, as shown in [Figure 3: see original paper] (b). [Figure 7: see original paper], [Figure 8: see original paper], and [Figure 9: see original paper] illustrate the trends of total energy, substitution formation energy, and stacking fault energy as functions of Y3 and Y2 element content.

[Figure 7: see original paper] Relationship between Y3 and Y2 element content and total energy of stacking fault mode S

As shown in [Figure 7: see original paper], for stacking fault mode S, refractory element doping reduces the system total energy, thereby improving system stability. For the system with Y3 replacing Al, the total energy gradually decreases with increasing dopant content, reaching its lowest value when Y3 content is approximately 4.2%. For the system with Y2 replacing Al, the total energy reaches its minimum when Y2 content is approximately 4.2%, then slightly increases with further Y2 addition. Thus, when Y2 content is approximately

4.2%, Y2 replacement yields the most stable system.

[Figure 8: see original paper] Relationship between Y3 and Y2 element content and substitution formation energy of stacking fault mode S

[Figure 9: see original paper] shows that both Y3 and Y2 doping can reduce the stacking fault energy. For the system with Y3 replacing Al, the stacking fault energy decreases rapidly as Y3 content increases from 0 to 1.4%, remains essentially constant when Y3 content is approximately 1.4% to 4.2%, and increases again when Y3 content exceeds 4.2%. The Y2 replacement system shows similar trends. Doping Y2 within a certain content range can reduce the stacking fault energy, consistent with previous researchers' conclusions. When dopant content is below 4%, the stacking fault energy of the Y3-replacing-Al system is always lower than that of the Y2-replacing-Al system. Combined with the analysis of total energy and substitution formation energy from [Figure 7: see original paper] and [Figure 8: see original paper], we can more definitively conclude that the Y3-replacing-Al system is the most stable.

Conclusions

Based on first-principles calculations of the γ/γ' binary model Ni-based single-crystal superalloy, we find that:

1. Doping with Y3 and Y2 elements can improve system stability. The system where Y3 and Y2 replace Al atoms in the γ/γ' binary model is more stable than when they replace Ni atoms, with the Y3-replacing-Al system showing the best stability. When Y3 and Y2 content is approximately 1.4%, the substitution formation energy is relatively low, and replacement of Al atoms occurs more readily.

2. Analysis of two different stacking fault modes reveals that as Y3 and Y2 content increases, the system total energy gradually decreases and stability improves. Compared with Y2 replacing Al, Y3 replacement yields better system stability and lower substitution formation energy. However, the Y3 content corresponding to optimal system stability with lowest substitution formation energy and stacking fault energy depends on the selected stacking fault mode.

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Note: Figure translations are in progress. See original paper for figures.