

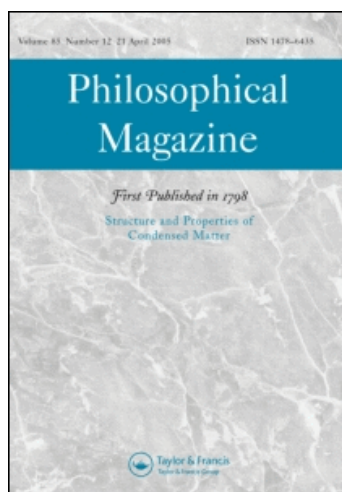
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Access details: Access Details: [subscription number 912295224]

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Philosophical Magazine

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title-content=t713695589>

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Online Publication Date: 01 November 2009

To cite this Article Wang, Yun-Jiang and Wang, Chong-Yu(2009)'Influence of alloying elements on the elastic properties of ternary and quaternary nickel-base superalloys',Philosophical Magazine,89:32,2935 — 2947

To link to this Article: DOI: 10.1080/14786430903140747

URL: <http://dx.doi.org/10.1080/14786430903140747>

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Influence of alloying elements on the elastic properties of ternary and quaternary nickel-base superalloys

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(Received 24 February 2009; final version received 23 June 2009)

Using new supercells, the influence of the alloying elements Co, Cr, Ta, Re, and Ru on the elastic properties of ternary and quaternary nickel-base superalloys are systematically studied by the first-principles pseudopotential method. The calculated results of the five ternary and three quaternary superalloys suggest that the alloying elements can increase the elastic moduli. Re is found to be most effective in increasing the moduli of ternary alloys. Among the quaternary alloys, the Ni-Al-Re-Ru system has the largest moduli. Our calculated values of the elastic moduli agree very well with the experimental results. The charge density redistribution and partial density of states are calculated for the quaternary system including both Re and Ru. Covalent-like bonding between Re and its nearest neighbor is observed. The hybridization between the Re-d orbital and the host Ni-p, d orbitals are the origin of the modulus strengthening effect.

Keywords: Ni-base superalloys; elastic property; alloying effect; first principles

1. Introduction

Nickel-base single crystal (SC) superalloys are a very important type of material, due to their superior elevated-temperature mechanical properties [1,2]. They are usually used in turbine blades for power generation and advanced aircraft engines. Superalloys are constituted by the precipitate γ' phase ($L1_2$, ordered face centered cubic (fcc), Ni_3Al based) and matrix γ phase (disordered fcc, solid solution based on Ni and with a random distribution of different alloying atoms). In general, it is the γ' phase which is largely responsible for the strength of the superalloys and their resistance to deformation. Modern commercial superalloys usually include more than a dozen alloying elements. The strengthening elements in the first generation superalloys contain Co, Cr, Ta, Mo, W, and so on. Further improvement in the overall performance of Ni-base SC superalloys requires more refractory elements, such as Re and Ru. The second and third generation superalloys contain about 3 wt% and 6 wt% of Re, respectively. Re has been proven to be a key element for the

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remarkable improvement of mechanical properties of superalloys [3–5]. However, excessive addition of refractory elements would lead to a tendency to form detrimental topologically packed phases (TCP). In order to suppress the precipitate of TCP, the element Ru is partially substituted for Re in the fourth generation Ni-base SC superalloys [6,7].

The elastic constants are important for a basic understanding of the mechanical properties of Ni-base superalloys. They have been measured previously by various methods [8–13]. However, as yet few direct experiments have been performed to examine the mechanical strengthening mechanisms of the elements alloying to Ni-base superalloys. At the moment, the strengthening mechanisms are not fully understood. Therefore, a deeper understanding of the influence of certain alloying elements on the elastic properties of superalloys is of great interest and should be systematically investigated. Experiments such as atom probe tomography (APT) and theoretical studies revealed that Co, Cr, Re, Ru all preferentially partition into the γ phase, whereas Ta has a strong tendency to partition into the γ' phase [14–18]. In view of the limitations of the experimental techniques, a first-principles approach has been extensively adopted to investigate the strengthening mechanisms related to these alloying elements, which are doped in both γ' phase and γ/γ' interface systems [19–23]. However, these studies were usually focused either on the site preference of alloying elements or an energetics study combined with electronic structures. This information is not sufficient to directly reflect the changes in elastic properties due to the additions. Moreover, the models in those papers are either clusters, or an interface with two vacuum layers, which cannot properly describe the fact that the γ' precipitate is surrounded by a γ matrix. A more reasonable Ni-base SC superalloys model is needed in the study of this field.

The objective of this paper is to systematically investigate the influence of the alloying elements Co, Cr, Ta, Re, Ru on the elastic properties of ternary and quaternary Ni-base SC superalloys using more reasonable supercell models. Because first-principles methods have achieved great success in studies on some mechanical properties of materials [24–27], we adopt them here for five ternary and three quaternary Ni-base superalloys to give a deeper understanding of the strengthening effect of alloying elements. The supercell models are constructed by a γ matrix surrounding γ' precipitates, which are more reliable compared to the previous studies. We present the calculated elastic properties of the model alloys and compare them with experiments. Furthermore, the electronic structures of quaternary Ni-Al-Re-Ru alloys are provided in detail as an example. This gives a concise insight into the reasons why the alloying elements slightly increase the elastic moduli.

2. Method and computational model

The first-principles calculations presented here are based on electronic density-functional theory (DFT), and have been carried out using the *ab initio* program VASP [28]. The generalized gradient approximation (GGA) using the Perdew–Wang (PW91) functional [29] of the projector augmented wave (PAW) method [30] is adopted for parameterization of the exchange-correlation functional. The cutoff energy of atomic wavefunctions is set to be 350 eV. Because the supercell in our paper

is large, k -points of only a $2 \times 2 \times 2$ mesh with a regular Monkhorst–Pack scheme are adopted. The convergence of energy with respect to the k -points is tested and a $2 \times 2 \times 2$ grid is enough. All the internal freedoms of supercell models are relaxed. The relaxation of the electronic degrees of freedom is stopped if the total energy change of the 256-atom supercell between two steps is smaller than 10^{-5} eV, while the coordinates of the atoms are fully relaxed when the total energy between two ionic relaxation steps is smaller than 10^{-4} eV.

The bulk modulus and elastic constants are evaluated by means of the total energies calculated as functions of suitable applied strains [26,31]. The theoretical equilibrium volume V_0 and bulk modulus B are determined by fitting the total energies versus volume according to the Murnaghan equation of state [32]. To get the cubic shear constants $C' = (C_{11} - C_{12})/2$ and C_{44} , we use the following volume conserving orthorhombic:

$$\varepsilon = \begin{pmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \frac{1}{(1+\delta)^2} - 1 \end{pmatrix}, \quad (1)$$

and monoclinic deformations:

$$\varepsilon = \begin{pmatrix} 1 & \delta/2 & \delta/2 \\ \delta/2 & 1 & \delta/2 \\ \delta/2 & \delta/2 & 1 \end{pmatrix}, \quad (2)$$

respectively. The corresponding total energies $E(0)$ and $E(\delta)$ are computed for 13 strains from $\delta = -0.03$ to $\delta = 0.03$ in steps of 0.005. The elastic constants C' and C_{44} are obtained by fitting the total energy-difference density with respect to δ as $\Delta E/V_0 = 6C'\delta^2 + O(\delta^3)$ and $\Delta E/V_0 = \frac{3}{2}C_{44}\delta^2$, respectively. Finally, the C_{11} and C_{12} elastic constants are separated from the bulk modulus $B = \frac{1}{3}(C_{11} + 2C_{12})$ and the shear constant C' .

The ternary and quaternary Ni-base SC superalloy models in the present work are based on the microstructure that the γ' precipitate is surrounded by the γ channels. The selection of our models is different from the previous first-principles calculations [21–23]. Compared to their cluster or interface models, our superalloy models are more reliable and closer to the microstructure of SC Ni-base superalloys. However, the real γ - γ' cube is the size of μm , which is much larger than that in our supercell model. Fortunately, the model with only 256 atoms is large enough to simulate the elastic properties of superalloys, since it is well accepted that the elastic properties of a two-phase material are only related to the volume fraction of the precipitate phase [33–36]. The volume fraction of the γ' phase in our models is about 56%, which is close to that of the experimental superalloys. Because the objective of this work is to qualitatively investigate the elastic properties of model alloys by alloying, structural defects such as dislocations and extended defects are excluded except for point defects.

The five ternary alloys in the present work are Ni-Al-X ($X = \text{Co}, \text{Cr}, \text{Ta}, \text{Re}, \text{Ru}$), while the three quaternary alloys include Ni-Al-Co-Cr, Ni-Al-Re-Ta and Ni-Al-Re-Ru. The distribution of alloying elements in these alloys is based on APT

experiments [14–16], which conclude Co, Cr, Re, Ru all partition preferentially to the γ matrix except for Ta. The segregation effect of the alloying elements near the interface is neglected. For the ternary alloys in this work, three Co (or Cr, Re, Ru) atoms uniformly substitute Ni atom in the γ phase, and simultaneously one substitutes the central Al atom in the γ' phase according to experimental results [14–16], while all four Ta atoms are sited uniformly in the γ' phase. For the quaternary alloys, there are altogether eight alloying atoms in our models: four for the first alloying element and four for the second element. The partition behavior of alloying atoms is also referred to in the APT experiments. The Ni-Al-Re-Ru quaternary alloy is shown in Figure 1 as an example. The large supercell model, including 256 atoms, is shown in Figure 1a. The central highlight part represents the γ' phase, which is a $3 \times 3 \times 3$ Ni_3Al unit cell alloyed with the colored additions. The outer part around the γ' phase is Ni alloyed with other elements, representing the γ solid solution. Here Figure 1a is one of the quaternary alloys, namely the Ni-Al-Re-Ru systems shown as an example. The other binary, ternary and quaternary alloys are also based on this structure. Figure 1b is the amplified γ' part belonging to the quaternary Ni-Al-Re-Ru alloys. The detailed atomic arrangement of one (100) layers in the model is shown in Figure 1c, which includes not only the host Ni and Al atoms, but also the alloying elements Re and Ru.

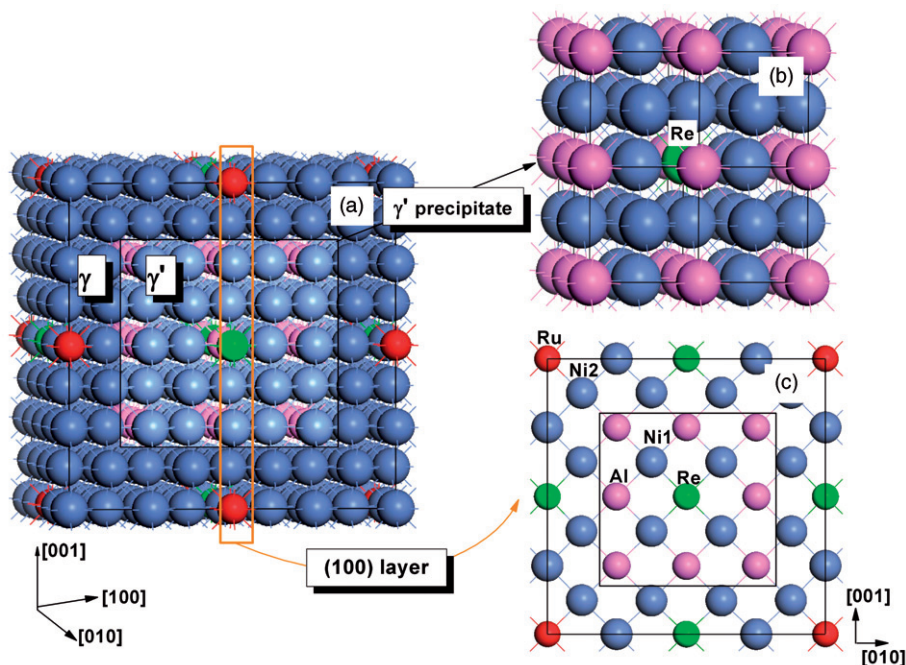


Figure 1. (a) The $4 \times 4 \times 4$ unit cells of the supercell of the quaternary γ/γ' Ni-base superalloys. The interior $3 \times 3 \times 3$ unit cells are $L1_2$ Ni_3Al phase, representing the γ' precipitate. The exterior part of the supercell is a Ni solid solution, representing the γ matrix. The blue and pink spheres are Ni and Al atoms. The green and red spheres are the alloying element Re and Ru. (b) The Ni_3Al precipitate alloying with Re. (c) A (100) plane of the supercell, which includes both the alloying elements Re and Ru.

3. Results and discussion

3.1. Effect of alloying elements on the elastic properties of superalloys

The chemical compositions of the five ternary and three quaternary Ni-base superalloys are listed in Table 1. The concentration of alloying elements in the alloys is referred to in the advanced commercial Ni-base superalloys. The lateral lattice parameters for both γ Ni and γ' Ni₃Al are kept the same for the assumption of coherence. First of all, the coherent lattice parameter and the bulk modulus B for the binary Ni-Al model alloy are determined by the Murnaghan equation of state. Here, the lattice parameter is defined as 1/4 width of the large supercell. The value is calculated to be 3.537 Å, which is between the lattice parameters of pure Ni (3.52 Å) and pure Ni₃Al (3.57 Å). For the ternary and quaternary alloys, the lattice parameters are all recalculated according to the energy–volume relations. We find that with Ta, Re, or Ru alloying atoms in the alloy, the lattice parameter increases, whereas, the Co and Cr additions have almost no effect on the lattice parameter. This result can be explained by the different sizes of the atomic radii between the host and alloyed atoms. Obviously, the elements of Ta, Re, and Ru have larger radii than the host atoms, while the radii of Co and Cr are smaller and comparable to those of the host atoms.

For the sake of understanding the strengthening effect of alloying elements on the elastic properties of Ni-base superalloys, the bulk modulus B and elastic constants C_{11} , C_{12} , C_{44} for the binary, ternary, and quaternary alloys are calculated. The results are listed in Table 2. For the binary Ni-Al alloy, the bulk modulus is 187.5 GPa, and the elastic constants are $C_{11} = 245.5$, $C_{12} = 158.5$, and $C_{44} = 112.9$ GPa, respectively. It is noticeable that the bulk moduli of all the ternary and quaternary alloys are larger than that of the binary alloy. From the results for ternary alloys, we notice that the alloying elements individually improve the bulk moduli of alloys with an order of Co < Ta < Cr < Ru < Re. The reason why Ta does not increase the bulk modulus as much as Ru and Re may have something to do with its γ' phase partition preference. This is consistent with the experimental fact that most of the solid solution strengthening elements partition preferentially to the γ matrix, and consequently improve the strength. Moreover, the elastic constants C_{11} and C_{44} for the ternary

Table 1. Chemical compositions of the five ternary and three quaternary alloys investigated in this study (wt.%). Addition 1 and Addition 2 are the first alloying element and the second alloying element, respectively.

Alloys	Ni	Al	Addition 1	Addition 2
Ni-Al-Co	77.6	19.4	3.0	
Ni-Al-Cr	77.9	19.5	2.7	
Ni-Al-Ta	72.4	18.9	8.6	
Ni-Al-Re	72.9	18.2	8.9	
Ni-Al-Ru	76.0	19.0	5.0	
Ni-Al-Co-Cr	75.8	19.2	3.0	2.0
Ni-Al-Re-Ta	66.7	17.0	8.3	8.1
Ni-Al-Re-Ru	70.0	17.8	8.7	3.5

Table 2. Calculated bulk modulus, elastic constants, Hill's shear and Young's modulus (in GPa), G/B ratio, Poisson's ratio ν of the binary, ternary, and quaternary Ni-base model superalloys at 0 K. The experimental values of two commercial Ni-base superalloys are also listed for comparison.

Alloys			B	C_{11}	C_{12}	C_{44}	G	E	G/B	ν
Binary	Ni-Al	Pre. work	188	246	159	113	77	203	0.411	0.319
Ternary	Ni-Al-Co		188	247	159	114	78	205	0.414	0.318
	Ni-Al-Cr		189	250	159	117	80	211	0.423	0.315
	Ni-Al-Ta		189	243	162	114	75	200	0.398	0.324
	Ni-Al-Re		191	253	160	119	81	214	0.426	0.314
	Ni-Al-Ru		190	250	160	117	80	210	0.419	0.316
Quaternary	Ni-Al-Co-Cr		190	251	159	117	80	211	0.422	0.315
	Ni-Al-Re-Ta		192	253	161	121	82	215	0.426	0.313
	Ni-Al-Re-Ru		193	256	161	124	84	220	0.437	0.309
Commercial alloys	TMS-26 ^a		189	252	159	132	87	227	0.460	0.300
	CMSX-4 ^b	Exp.	190	251	159	132	87	225	0.456	0.302

^aRef. [8], measured at room temperature with the resonance ultrasound spectroscopy method.

^bRef. [11], measured at room temperature with surface Brillouin scattering.

alloys increase, but Ta is an exception. However, C_{12} behaves differently. The strengthening effect order for C_{12} in ternary alloys is $\text{Cr} < \text{Co} < \text{Ru} < \text{Re} < \text{Ta}$. The reason is that the C_{12} of γ' phase is larger than that of the γ phase, which is opposite to C_{11} and C_{44} . The alloyed Ta atoms in our ternary alloys are distributed in the γ' phase, which results in an alloying effect on γ' and enlarges the value of C_{12} .

The modulus strengthening effect of alloying elements on the ternary alloys can also be seen in the quaternary alloys. When alloying with (Co, Cr), (Re, Ta) or (Re, Ru), the bulk modulus and elastic constants of quaternary alloys increase. Among them, the Ni-Al-Re-Ru quaternary system has the largest mechanical strength compared to the Ni-Al binary alloy. In Figure 2, we show the $\Delta E/V_0\text{-}\delta$ relation fitted by a second-order polynomial to determine C_{44} as an example. The alloying elements in the ternary and quaternary alloys are Re and Ru, respectively. From the figure, we can see clearly that Re (or Ru) individually increases C_{44} . The strengthening effect of Re is more obvious than Ru. When alloying with both Re and Ru, the alloy has the largest elastic moduli.

Besides the bulk modulus and elastic constants, the shear modulus is calculated as the arithmetic Hill average [35] $G = \frac{1}{2}(G_V + G_R)$, where $G_V = (C_{11} - C_{12} + 3C_{44})/5$ and $G_R = 5/(4S_{11} - 4S_{12} + 3S_{44})$ are the Voigt and Reuss bounds, respectively, and S_{11} , S_{12} , and S_{44} are the elastic compliances. Finally, Young's modulus E and Poisson's ratio ν are obtained as $E = 9GB/(G + 3B)$ and $\nu = \frac{1}{2}(3B - 2G)/(3B + G)$, respectively. The results are also listed in Table 2. It can be seen that with alloying elements, the shear and Young's modulus both increase. The Ni-Al-Re-Ru quaternary model alloy has the largest moduli, which is consistent with the increase in bulk modulus and elastic constants. The obvious increments in G and E are approximately 9% and 8%, respectively. On the other hand, the increase in elastic moduli may be accompanied by increased brittleness. According to Pugh's empirical

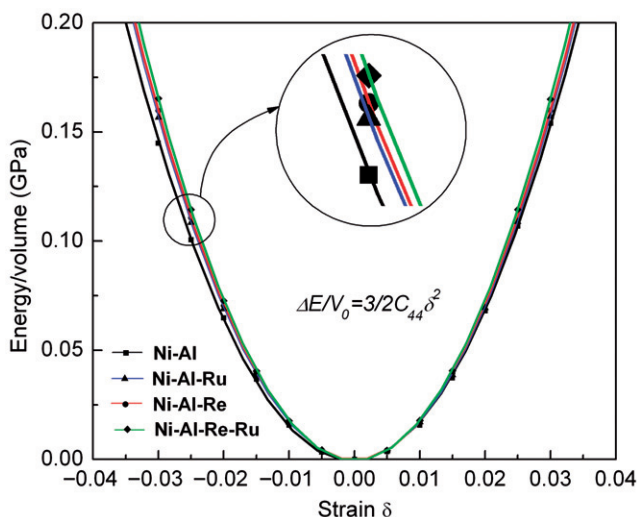


Figure 2. (Color online). The strain-energy density variation relations fitted by $\Delta E/V_0 = \frac{3}{2} C_{44} \delta^2$. The black square, triangle, circle and diamond represent binary Ni-Al, ternary Ni-Al-Ru, Ni-Al-Re, and quaternary Ni-Al-Re-Ru alloys, respectively.

rule [39], the ductile/brittle behavior of the material is closely related to the ratio of G/B or Poisson's ratio ν . A high value of G/B and a low value of ν is associated with brittleness. The increase in G/B or decrease in ν indicates a decrease in ductility. It is interesting to notice from the G/B and ν values listed in Table 2 that the alloys indeed become more brittle with alloying. However, it should be pointed out that the G/B value of both the model alloys and commercial alloys lies between about 0.4 and 0.46, which is still far from 0.57, the value to separate ductile and brittle material [39]. Therefore, the Ni-base alloys can still be regarded as ductile material. In other words, the increased brittleness in ternary and quaternary alloys with alloying can be tolerant in applications.

Moreover, it is interesting to know the effect of magnetism on the elastic properties of alloys from the ferromagnetic property of Ni atom. Among all the model alloys in our calculations, we take binary Ni-Al and quaternary Ni-Al-Re-Ru as examples to see how the magnetism affects the elastic properties. The calculated magnetisms for binary Ni-Al and quaternary Ni-Al-Re-Ru alloys are $0.33 \mu_B$ and $0.29 \mu_B$ per atom, respectively. As predicated, the magnetism of the alloy is partly lost with alloying. The calculated elastic constant C_{44} for the Ni-Al alloy with spin polarization is 117.6 GPa, which increases by about 4% with respect to the non-spin-polarized value of 112.9 GPa, whereas the corresponding values for Ni-Al-Re-Ru are 124.7 GPa and 123.4 GPa, respectively. The spin-polarized value for C_{44} is 1% larger than the non-spin-polarized value. The result indicates that magnetism affects the elastic properties of Ni-base model alloys. Taking magnetic ordering into consideration, the elastic moduli are larger than those without spin polarization. However, the relative order of elastic moduli of different systems is not reversed. Therefore, the calculated moduli are still reliable to qualitatively compare the elastic properties of alloys with and without alloying.

Finally, in order to confirm the reliability of our method for the calculations of elastic properties for Ni-base model alloys, we compare the calculated results with the experimental measurements of the second generation Ni-base SC superalloys CMSX-4 [11] and the fourth generation one TMS-26 [8]. Our calculated elastic moduli of model alloys agree very well with the experimental results. With the exception of C_{44} , the difference between the calculated and experimental values is negligible. It should be pointed out that the errors in the elastic moduli derived from the fitting of the total energy to the strain magnitude are within 0.6%, while the errors in the measured elastic moduli of commercial alloys are of the order of 1%. In the next part, we will present the electronic structure of the Ni-Al-Re-Ru quaternary alloy in detail. The analysis will provide a deeper understanding of why these alloying elements increase the elastic moduli of superalloys.

3.2. Electronic structure

3.2.1. The charge density redistribution

In this section, we study the electronic mechanisms of the alloying effect on Ni-base SC superalloys. Here the quaternary Ni-Al-Re-Ru alloy is taken as an example to show the origin of the modulus strengthening effect. Figure 3 shows the total valence charge density difference on a (100) plane corresponding to Figure 1c at different strains. The plane includes alloying atoms Re in both the γ and γ' phases, and Ru in the γ phase. The charge density difference is defined as the difference between the self-consistent charge density of the system and the superposition of the free atom density. Figures 3a, c and e are the charge differences of alloying atom Re and its neighbors, and the strains correspond to $\delta = 0, 0.015, 0.030$. The strain configuration corresponds to the monoclinic deformation shown in Equation (2). The charge difference of Ru addition together with its neighbors is shown in Figures 3b, d and f. It can be seen that charge correction regions due to electron accumulation appear around Re (and Ru), and their nearest neighbor (NN) Ni atoms. This indicates that there exists a strong interaction between alloying atoms and their NNs. We can also see that the bonding between Re and its NNs is stronger than that of Ru. Furthermore, the charge difference between Re and its NNs takes on a covalent-like character. The bonding has an obvious directional distribution. The covalent-like bonding varies little from strain $\delta = 0$ to $\delta = 0.03$. One can believe that it is this feature of Re bonding that leads to the contributions to its shear moduli. As the material deforms, it should overcome the strong directional bonding. This is consistent with the result that Re is the most effective addition for the modulus strengthening of alloys. In contrast with Re, we notice that the shape of the charge correction region of Ru has different features. The charge accumulation around Ru is spherically symmetric near the atomic site, which is in qualitative agreement with the picture of metallic bonding. Moreover, we find the charge redistribution around Ru accumulates more and more in one of the Ni-Ru-Ni directions as the material deforms. The uniform redistribution of charge is gradually broken with deformation. Conclusively, this feature of the Ru charge redistribution is not as effective as Re in preventing the deformation of the material. This is the reason why

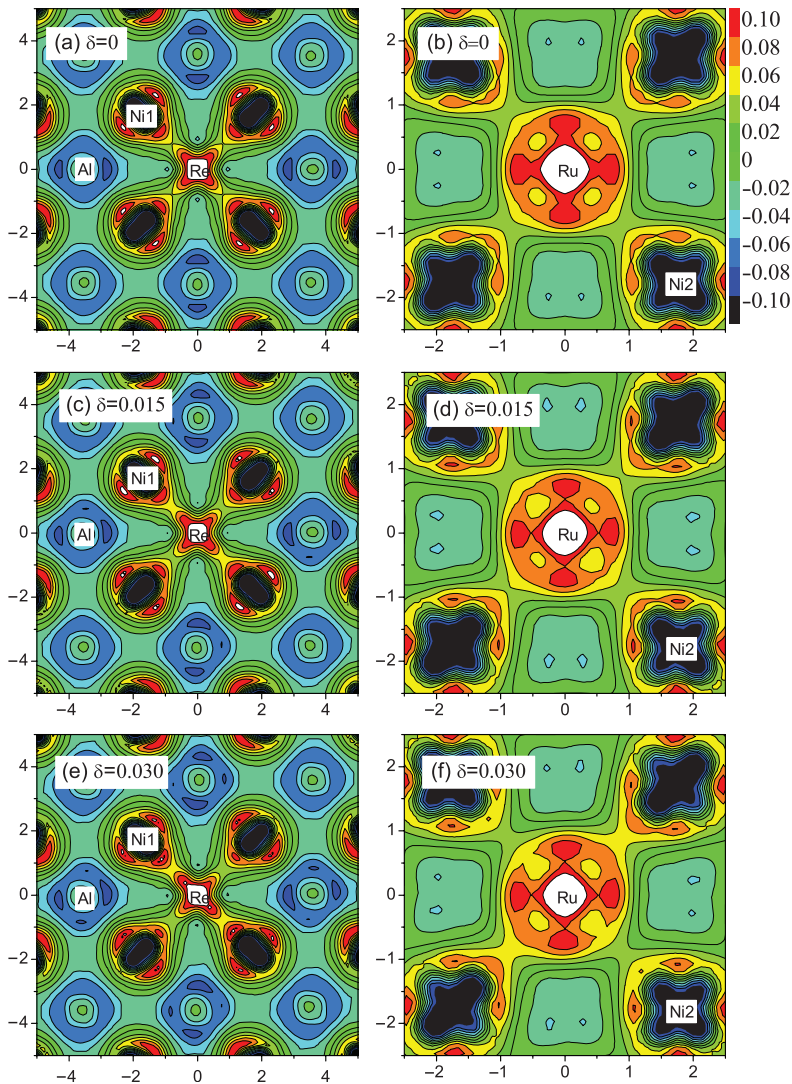


Figure 3. The charge density difference on the (100) planes at different shear strains $\varepsilon = 0, 0.015, 0.030$ from quaternary Ni-base superalloy alloyed with Re and Ru. Positive (negative) values denote charge accumulation (depletion).

the alloying of Re increases the modulus more effectively than Ru. Based on the above analysis, the bonding feature between Re (Ru) and the host atoms effectively strengthens the material. On the other hand, according to the increased values of G/B , the material becomes more brittle, which follows from the more pronounced covalent component of the interatomic bonding. It can also be expected that the synthetic alloying effect of both Re and Ru would be better than their individual ones.

3.2.2. Partial density of states

Besides charge redistribution, the atomic Partial Density of States (PDOS) of Re, Ru and their neighbors in the quaternary Ni-Al-Re-Ru alloy are provided in Figure 4. All the atoms shown here are located on the (100) plane corresponding to Figure 1c. Figure 4a is the PDOS of alloying atom Re and its NN Ni1, and second NN Al are included as well. Figure 4b shows the PDOS curves for Ru and its NN Ni2. It can be

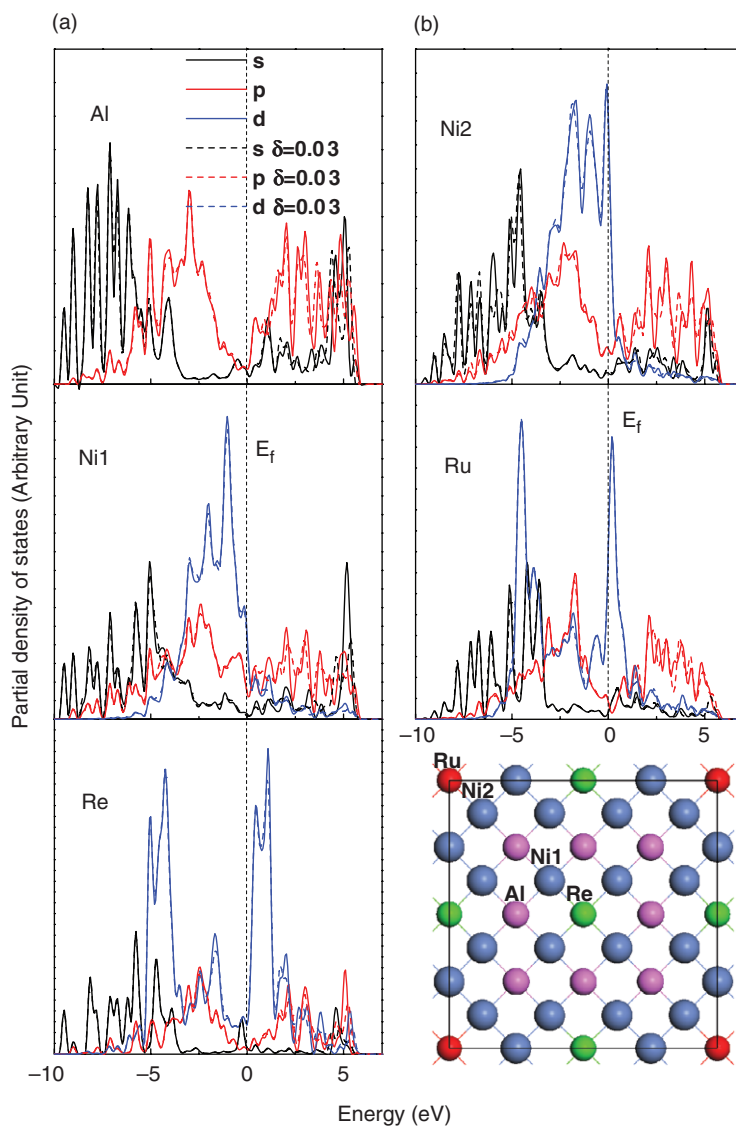


Figure 4. (Color online). The atomic partial density of states of the alloying elements Re and Ru and their nearest neighbors and the second nearest neighbors. The Fermi levels are shifted to zero. The solid lines represent the PDOS curves of atoms at equilibrium, while the dashed lines are those at a shear strain of $\delta = 0.03$.

seen from Figure 4a that Al-3s, 3p orbitals hybridize with Ni1-4s, 4p orbitals, which leads to the energy bands smearing out over the whole energy range. In contrast with the host atoms Al, a deep valley separates the bonding and antibonding regions of the PDOS for the alloying elements Re, in which the Fermi level is located in the valley, indicating that the substitution stabilizes the superalloy [37]. This feature of the Re PDOS also indicates a strong interaction between the doped element and the host atoms, suggesting higher moduli [38]. The origin of the strong bonding between Re and Ni1 is that the Re-d orbital hybridizes strongly with the s, p, and d states of Ni1; in contrast, there is no d orbital in host Al atoms, thus the interaction between Re and Al is weak. There exist two resonant peaks between Re and Ni1: one is Re-d, Ni1-p at -5 eV , and the other is Re-d, Ni1-s at -4.3 eV below the Fermi level. It is also interesting to see in Figure 4b that the Ru-d orbital hybridizes with its NN Ni2-s, p states. The main resonant peak is Ru-d and Ni2-p located at -4.5 eV below the Fermi level. Compared to Re, there are some isolated PDOS peaks of Ru appearing on both sides of the Fermi level, resulting in the alloying effect not being as strong as Re. In Figure 4, the PDOS of alloying atoms and their neighbors at strain $\delta=0.03$ are also plotted as dashed lines. We find that the d orbitals of atoms remain nearly unchanged with strains. Moreover, the s, p curves of bonding states are affected little by the strain, although the antibonding states are adjusted. This shows that the alloying elements can effectively prevent the alloy from deforming. The PDOSs here are consistent with the analysis of the charge redistribution. They both indicate that when alloying with Re and Ru, the elastic moduli of alloys are increasing. The effects of Re are stronger than those of Ru.

4. Summary

In summary, we have systematically investigated the influence of alloying elements on the elastic properties of Ni-base SC superalloys for five ternary and three quaternary model superalloys. The present first-principles study adopts a new structure of the supercell, which is a γ' phase surrounded by the γ matrix. It is more reliable than previous investigations because the microstructure is closer to real Ni-base superalloys. The ternary alloys are Ni-Al-X ($X=\text{Co, Cr, Ta, Re, Ru}$) systems, while the quaternary ones include Ni-Al-Co-Cr, Ni-Al-Re-Ta and Ni-Al-Re-Ru. The distribution of alloying atoms in our model is based on atom probe experiments. Based on the calculated results, we find that almost all the additions increase the elastic moduli of model alloys. Among them, Re is the most effective element in strengthening the ternary model alloys. For the quaternary model alloys, Ni-Al-Re-Ru has the highest elastic moduli. Our calculated values of elastic moduli compare well with the experimental values of commercial Ni-base SC superalloys. The electronic structures of Ni-Al-Re-Ru systems are provided as an example to explain the moduli strengthening effect. Strong charge accumulation (depletion) regions appear around Re and Ru. The covalent component of bonding between Re and its NN increases the resistivity of the material against deforming and leads to higher values of the elastic constants, but also induces increased brittleness, while the metallic bonding feature between Ru and its NNs makes the strengthening effect not as strong as Re. The analysis of PDOS curves for Re, Ru and their

neighbors leads to the same conclusion. The strong hybridization between Re-d (Ru-d) orbitals and NN Ni-s, p states is the origin of the alloying effect on alloys.

Acknowledgement

A financial grant of the '973 Project' (Ministry of Science and Technology of China, Grant No. 2006CB605102) is gratefully acknowledged.

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