Energetics and electronic structure of refractory elements in the dislocation of NiAl*

Chen Li-Qun(陈丽群)[a)†], Peng Xiao-Fang(彭小方)[a)], and Yu Tao(于 涛)[b)]

[a)] *College of Sciences, Central South University of Forestry & Technology, Changsha* 410004, *China*
[b)] *Central Iron and Steel Research Institute, Beijing* 100081, *China*

(Received 12 January 2012; revised manuscript received 12 February 2012)

Using DMol and the discrete variational method within the framework of the density functional theory, we study the alloying effects of Nb, Ti, and V in the [100] (010) edge dislocation core of NiAl. We find that when Nb (Ti, V) is substituted for Al in the center-Al, the binding energy of the system reduces 3.00 eV (2.98 eV, 2.66 eV). When Nb (Ti, V) is substituted for Ni in the center-Ni, the binding energy of the system reduces only 0.47 eV (0.16 eV, 0.09 eV). This shows that Nb (Ti, V) exhibits a strong Al site preference, which agrees with the experimental and other theoretical results. The analyses of the charge distribution, the interatomic energy and the partial density of states show that some charge accumulations appear between the impurity atom and Ni atoms, and the strong bonding states are formed between impurity atom and neighbouring host atoms due mainly to the hybridization of 4d5s(3d4s) orbitals of impurity atoms and 3d4s4p orbitals of host Ni atoms. The impurity induces a strong pinning effect on the [100] (010) edge dislocation motion in NiAl, which is related to the mechanical properties of the NiAl alloy.

Keywords: electronic structure, dislocation, intermetallic compounds, impurity

PACS: 71.15.Mb, 71.55.Ak, 61.72.Lk, 61.72.sh **DOI:** 10.1088/1674-1056/21/8/087102

1. Introduction

Mechanical properties of the intermetallic compound NiAl such as high strength, good corrosion resistance and high melting temperature are of great interest due to its application in the aerospace industry. However, the weak high temperature creep resistance and room temperature brittleness are well known as two principal problems which restrict its wide applications. Consequently, improving its ductility has been tried using many techniques and of these, microalloying seems to be the most promising approach.[1] Some investigations[2−5] have shown significant improvement on the fracture toughness and creep resistance of NiAl/X eutectic composite with refractory metal reinforcement. However, the mechanical properties of the material are influenced by many factors such as impurity content and constitutional defects. It is well known that the brittleness in NiAl-based material has been attributed to the lack of sufficient independent slip systems. The a[100] deformation mode results in only three independent slip systems, and consequently, the room temperature tensile ductility of NiAl is almost nil.[6] Takasugi *et al.*[7] reported on unexpected high elongations (100%–350%) of NiAl single crystals at intermediate temperature and soft orientations. It was found that the deformation mechanism of this phenomenon is the hardening from forest dislocations with thermally activated cross-slip events.[8−11] Pollock *et al.*[12] also found that NiAl deforms by glide of [100] dislocations. Therefore, the nature of elementary impurity-dislocation interaction is one of the key questions in the physics of the strength and plasticity of solid solution.

Although the impurity–dislocation interaction depends on many factors and according to the prevailing point of view, the size misfit between the impurity and host atoms appears to make the main contribution in the majority of alloys. On the other hand, there are a number of cases where the electronic structure of the impurity plays a more important role than the size misfit. The mechanical properties of a NiAl compound depend crucially on the microalloying addition. Firstly, an alloying atom locally changes the electronic structure and bonding characteristics of the compound. This, in turn, can influence the energy characteristics determining the fracture behaviour and the dislocation mobility.[13] Kontsevoi *et al.*[14] calculated

*Project supported by the National Basic Research Program of China (Grant No. 2011CB606402).
†Corresponding author. E-mail: ldclqun@163.com
© 2012 Chinese Physical Society and IOP Publishing Ltd

the local densities of states and energy of NiAl with a[100] (010) edge dislocation and transition-metal impurities (Ti, V) using the real-space tight-binding linear muffin-tin orbital method. The localized electronic states, appearing in the core of the dislocation, are found to lead to strong impurity-dislocation interaction via two mechanisms: firstly, chemical locking, due to strong hybridization between impurity electronic states and dislocation localized states; secondly, electrostatic locking, due to long-range charge oscillations caused by the electron localization in the dislocation core. The results obtained explain qualitatively why the solid-solution hardening effect in NiAl correlates with the electronic structure of impurities rather than with size misfit. Recently, Chen and Yu[15] investigated the boron-dislocation interaction in NiAl. The results show that B forms strong bonding states with its neighbouring host atoms, so it can be expected that the strength of NiAl may be increased.

To our knowledge, there is a lack of studies on the interaction between dislocation and impurity in the NiAl alloy at an electronic level. Kontsevoi *et al.*[14] calculated only the local densities of states and energy of NiAl with a[100] (010) edge dislocation and transition-metal impurities (Ti, V). On the other hand, we also intend to understand the effect of 4d metal impurity on the edge dislocation of NiAl. Therefore, in the present work, we investigate the effects of impurities (Nb, Ti, and V) on the electronic structure of [100] (010) edge dislocation in NiAl (We select the [100] (010) edge dislocation, because almost all of the dislocations in NiAl have Burgers vectors with $b = \langle 100 \rangle$, and most of the dislocations are on the edge [16,17]), and calculate the impurity segregation energy, the interatomic energy, the charge density, and the density of states. First, we perform structure optimization of the [100] (010) edge dislocation core with impurities using the DMol[18,19] method. Then, the electronic structures of the dislocation core with and without impurities are calculated, respectively, by the discrete variational method (DVM).[20,21]

2. Method and model

In the DMol method, the energy gradient for each atom can be calculated conveniently, and the desired equilibrium atomic structure and the total energy of the ground state can be obtained by relaxing the atom until the forces acting on the atom become zero. It is convenient to use the cluster model for exploring the site distortion and electronic properties of the local defect system. The cluster model used in the DMol calculation is generated from the atomic configuration obtained by a molecular dynamics relaxation[15] with Voter–Chen-type potential.[22] The molecular dynamics method is widely used in the static and dynamic simulation of material structure and property.[23−25] Figure 1 shows the cluster model for [100] (010) edge dislocation. The atoms denoted by solid and open circles construct alternate (001) crystal planes (denoted as A and B, respectively) and are stacked consecutively. Because the atoms in A plane are either Ni atoms or Al atoms, two different dislocation core (DC) centres are formed, and these will be referred to as centre-Ni and centre-Al, respectively. The models of centre-Ni and centre-Al have AlNiAlNiAlNiAl and NiAlNiAlNiAlNi stacking sequences along the [001] direction, respectively, with a total of 209 atoms. Considering the impurity site preference and symmetry of model, the impurity Nb (Ti and V) is placed at the position labeled 1 (see Fig. 1), substituted for the corresponding Al atom in the centre-Al and Ni atom in the centre-Ni, respectively. Then we performed the structure optimization for [100] (010) edge dislocation with impurity Nb (Ti, V) by using DMol. During the optimization, the impurity atom Nb (Ti, V) and the neighbouring atoms (all the atoms labeled by the numerals in Fig. 1) are fully relaxed. The relaxation results in a configuration with C_{2v} symmetry. The optimized geometry structure is obtained within the tolerances of 0.0001 Ry/a.u and 0.00005 for the gradient convergence and the electron density convergence, respectively.

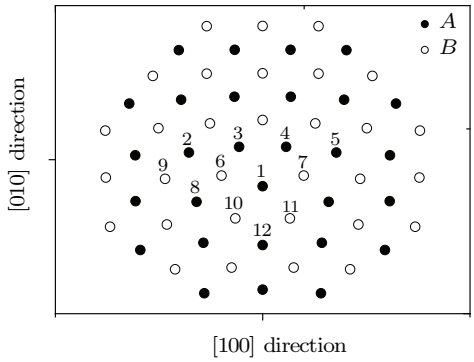


Fig. 1. Atomic model of the [100] (010) edge DC in NiAl. Atoms denoted by solid circles and open circles construct two adjacent planes (plane A and plane B, respectively) in the stacking sequence along [001].

We employ the first-principles DVM based on density functional theory and local density approximation to calculate the electronic structure of the

dislocation core in NiAl. This method has been successfully used to study electronic structures of metals, alloys, and intermetallic compounds.[26,27] The molecular orbitals are expressed as a linear combination of atomic orbitals, and the single site basis set with the frozen core mode is used in the atomic orbitals. The Coulomb potential is calculated in the self-consistent charge approximation, and the exchange–correlation potential takes von Barth and Hedin type.[28] In the computation, the convergence is accepted if the root-mean-square of all atomic orbital populations differs by less than 10^{-5} between two successive iterations.

3. Results and discussion

3.1. Energy analysis

We introduce the impurity segregation energy ($E_{\rm seg}$) to discuss the energy change caused by Nb (Ti, V). $E_{\rm seg}$ is defined as[29]

$$E_{\rm seg} = \frac{E_{\rm b}^{\rm dop} - E_{\rm b}^{\rm clean}}{N}, \tag{1}$$

where $E_{\rm b}^{\rm dop}$ and $E_{\rm b}^{\rm clean}$ are the binding energies of the impurity-doped system and the clean system, respectively. N is the total number of impurity atoms in the impurity-doped system. Using the DMol method, we calculate the binding energy $E_{\rm b}$ and impurity segregation energies $E_{\rm seg}$ of Nb, Ti, and V in the [100] (010) edge dislocation of NiAl for two models of centre-Ni and centre-Al, respectively. The calculated results are listed in Table 1. Apparently, the doped DC system displays a low binding energy compared with the clean DC system. It suggests that the doped DC systems are more stable than the clean DC system. The $E_{\rm seg}$ in the centre-Al is much lower than that in the centre-Ni, indicating that the impurity Nb (Ti, V) prefers to occupy the centre-Al DC rather than the centre-Ni DC. That is, the Nb (Ti and V) impurity occupys the Al sublattice in NiAl. The result is in agreement with the results of previous experimental [30,31] and theoretical calculations.[14,32] In fact, the atomic radii of Nb, Ti, and V are very close to that of Al, but quite different from that of Ni (the atomic radii of Nb, Ti, V, Al, and Ni are 1.47 Å, 1.47 Å, 1.36 Å, 1.43 Å, and 1.25 Å, 1 Å= 0.1 nm respectively). Therefore, from the point of view of atomic size, Nb, Ti, and V would prefer to occupy an Al site, and not induce a severe local lattice distortion in the [100] (010) edge dislocation of NiAl. We calculate only the electronic structures of the centre-Al DC with and without impurity Nb (Ti, V). In addition, the impurity segregation energies of the three elements (Nb, Ti, V) are different, in the increasing order Nb<Ti<V. It is thus evident that Nb and Ti are energetically more favourable to the stabilization of the system of NiAl than V. The trapping effect of the dislocation core on impurities will potentially influence the dislocation mobility, as a result, which will affect the macroscopic properties of NiAl.

The interatomic energy (IE) is a measurement of the interaction between two atoms. For the l-th and m-th atoms, it is derived as[33,34]

$$E_{lm} = \sum_{n} \sum_{\alpha\beta} N_n a_{n\alpha l}^{*} a_{n\beta m} H_{\beta m \alpha l}, \tag{2}$$

where N_n is the occupation number for molecular orbital ψ_n, $a_{n\alpha l} = \langle \phi_{\alpha l}(r) | \psi_n(r) \rangle$, and $H_{\beta m \alpha l}$ is the Hamiltonian matrix element connecting the atomic orbital β of atom m and the atomic orbital α of atom l. Since the IE is related to the Hamiltonian matrix element, it can be used to estimate the bonding capability of the two atoms. Usually, a negative number with a large absolute value means a strong interatomic interaction. Table 2 presents the IEs of some interesting atomic pairs for the doped DC system and the clean DC system. In order to show the effect of the alloying addition clearly, the changes of IEs induced by the substitution of an impurity atom for Al are also presented.

From Table 2 it can be found that the IEs between the impurity atom and its neighboring host atoms are strongly increased except for the Nb1–Al3 atomic pair, which means that the impurity atom substitution can enhance the bonding between atoms compared with the clean DC system. Table 2 also shows that the bond strengths between the host atoms increase in the

Table 1. Values of binding energy ($E_{\rm b}$) and impurity segregation energy ($E_{\rm seg}$) (in eV) in the DC system.

Energy	Center-Ni DC				Certer-Al DC			
	Clean	Nb-doped	Ti-doped	V-doped	Clean	Nb-doped	Ti-doped	V-doped
$E_{\rm b}$	–714.98	–715.45	–715.14	–715.07	–668.59	–671.59	–671.57	–671.25
$E_{\rm seg}$		–0.47	–0.16	–0.09		–3.00	–2.98	–2.66

Table 2. Interatomic energies (in eV) for selected atomic pairs in the dislocation core with and without impurities. $\Delta E_{\rm Nb}$, $\Delta E_{\rm Ti}$, and $\Delta E_{\rm V}$ are obtained by subtracting the IE in the clean DC from the IE in the doping DC, respectively. Atom 1 denotes an Al atom in the clean DC and impurity atoms (Nb, Ti, V) in the doping DC, respectively. The Arabic numbers correspond to those in Fig. 1.

Atomic pairs	Clean IE	Nb-doped IE	$\Delta E_{\rm Nb}$	Ti-doped IE	$\Delta E_{\rm Ti}$	V-doped IE	$\Delta E_{\rm V}$
Atom1–Ni6	–1.35	–1.65	–0.30	–1.54	–0.19	–1.66	–0.31
Atom1–Ni10	–1.03	–1.43	–0.40	–1.70	–0.67	–1.68	–0.65
Atom1–Al3	–0.71	–0.66	0.05	–0.75	–0.04	–0.97	–0.26
Atom1–Al12	0.02	–0.09	–0.11	–0.27	–0.29	–0.14	–0.16
Al3–Al4	–1.50	–2.07	–0.57	–1.90	–0.40	–1.92	–0.42
Ni6–Ni9	–0.70	–0.86	–0.16	–0.80	–0.10	–0.78	-0.08
Ni10–Ni11	–0.93	–1.08	–0.15	–1.00	–0.07	–1.09	-0.16

doping impurity systems. In particular, the interactions between the impurity atom and the nearest-neighbouring host atoms (Ni6, Ni10) are much stronger than those between the Al1 atom and corresponding host atoms in the clean DC. This shows that the impurity atoms form strong bonds with the adjacent host atoms. Therefore, the motion of DC with the impurity atom is harder than that of a clean dislocation line. That is, the impurity atom can greatly enhance the interaction between the atoms in the DC. This mechanism will contribute strongly to the solid-solution hardening. In addition, the interactions between the atoms in the DC are different for three doping impurity systems. The IEs between the V1 atom and its adjacent host atoms are strongest, Nb1 weakest and Ti1 medium. However, the IEs between the host atoms are strongest in the Nb-doped system, weakest in the Ti-doped system, and medium in the V-doped system.

3.2. Charge distribution

In order to gain further insight into the physical origin of the influence of alloying atoms on the mechanical properties of NiAl, we draw the charge density difference of the doping impurity DC systems. The charge density difference is defined as follows:

$$\Delta\rho_{\rm imp} = [\rho\,({\rm dis_{sub}}) - \rho_{\rm free}\,({\rm dis_{sub}})] - [\rho\,({\rm dis_{clean}}) - \rho_{\rm free}\,({\rm dis_{clean}})]\,, \quad (3)$$

where $\rho\,({\rm dis_{sub}})$ and $\rho_{\rm free}\,({\rm dis_{sub}})$ are the charge densities of the bonding atom system and the free atom system for the impurity substituted dislocation system ($\rm dis_{sub}$), while $\rho\,({\rm dis_{clean}})$ and $\rho_{\rm free}\,({\rm dis_{clean}})$ are the charge densities of the bonding atom system and the free atom system for the clean dislocation system ($\rm dis_{clean}$), respectively. We will refer to $\Delta\rho_{\rm imp}$ as the impurity-induced charge density. $\Delta\rho_{\rm imp}$ in the (001) plane containing impurity atom Nb (Ti, V) is shown in Fig. 2. Figure 3 shows $\Delta\rho_{\rm imp}$ in the (100) plane which contains the impurity atom Nb (Ti, V).

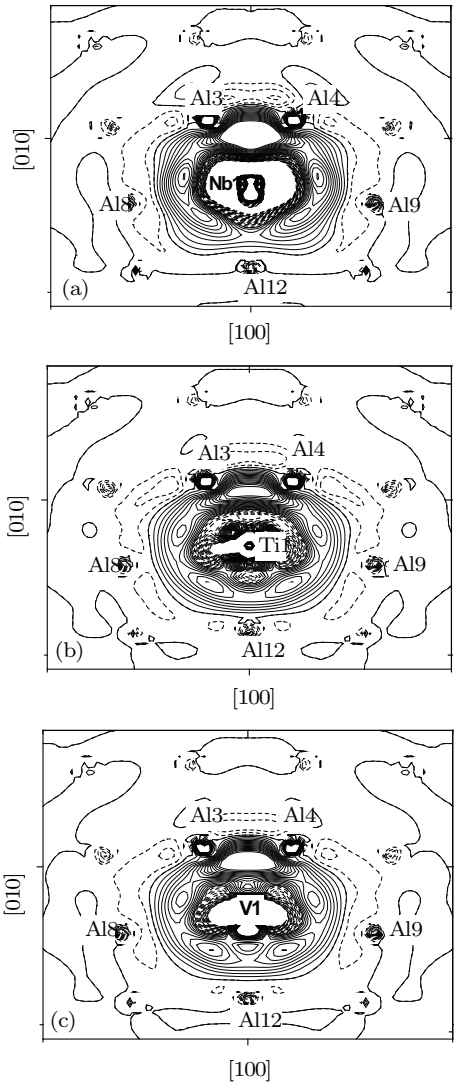


Fig. 2. Charge density difference of doped DC for the central plane A. The contour spacing is $0.002{\rm e}/({\rm a.u})^3$. Solid (dashed) lines mean a gain (loss) of charge: (a) the Nb-doped DC; (b) the Ti-doped DC; (c) the V-doped DC.

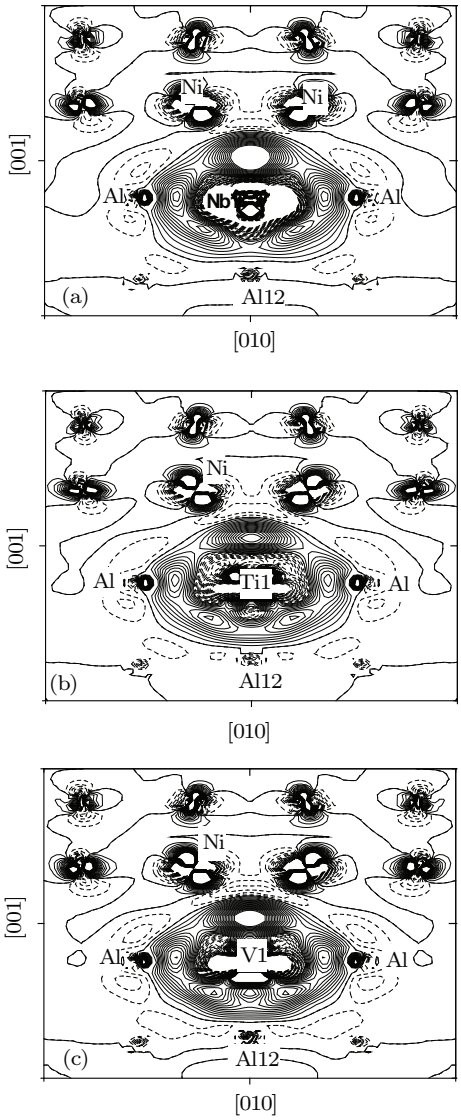


Fig. 3. The charge density difference in the (100) plane containing the impurity atom. The contour spacing is $0.002e/(a.u)^3$. Solid (dashed) lines mean a gain (loss) of charge: (a) The Nb-doped DC; (b) the Ti-doped DC; (c) the V-doped DC.

From Fig. 2, pronounced charge redistributions can be observed for three impurity-substituted systems. The charges accumulate mainly between the impurity atom and the neighbouring host atoms (Al3, Al4, Al8, and Al9), which means that the strong chemical bonding between the impurity atom and neighbouring Al atoms is formed. A common feature is that the interactions between the impurity atom and Al atoms are localized within a small region.

From Fig. 3, we can also see that for the three impurity-substituted systems, there is a charge accumulation between the impurity atom and the neighbouring host atoms. This implies that the interactions between the impurity atom and the host atoms (Ni, Al) along the dislocation line direction are also enhanced. The above charge density analyses reflect the strong pinning effect of the impurity atoms on the [100] (010) DC motion, which should affect the mechanical properties of NiAl alloys.

3.3. Density of states

The density of states is closely related to the bonding character between atoms. In order to analyse the interaction between the impurities and host atoms further, we calculate the partial density of states (PDOS). Figures 4(a)–4(d) show the PDOS curves for atom 1 (atom 1 denotes the Al1 atom and the impurity atom in the clean dislocation system and impurity-substituted system, respectively) and the neighbouring host atoms (Al3, Ni6, Ni10). Two atomic bonding features have been previously observed in Fig. 4. Compared with the case of the clean DC system, the PDOS curves of Ni10, Ni6, and Al3 shift towards the lower energy in the impurity-substituted system. This means that some itinerant electrons are transferred to some deeper energy levels in the valence band, and participate in bonding with the impurity atom Nb (Ti, V). In addition, we can see from Fig. 4(a) that the Al1-3s3p orbitals hybridize with the Ni6(Ni10)-4s4p orbitals, as well as the Al3-3s3p orbitals, which have a weak interaction with the 3d orbitals of the Ni atom (Ni6, Ni10). In the three impurity-substituted systems, the PDOS curves of the Ni6 (Ni10)-4s4p orbitals considerably change in the regions of the bonding states and antibonding states. While the PDOS curves of the Ni-3d orbitals hardly change. The local feature of the Ni-3d state remains intact, and exhibits a single peak structure over a range of about -13 eV–-7 eV. From Figs. 4(b)–4(d), we can find that Ni-4s and Al-3s orbitals show up primarily as the characteristic peak structure in a low energy range from -19 eV to -10 eV. Meanwhile, the 5s (4s) orbitals of impurity atom Nb (Ti, V) each have a resonant peak with the 3d orbitals of the Ni6 (Ni10) atom at about -12.6 eV. This is an indication of strong hybridization between the impurity electronic states and the Ni electronic states, showing that there is a strong chemical interaction between the impurity atom and neighbouring host Ni atoms. On the other hand, the 3d4s4p orbitals of the Ni6 (Ni10) atom and the 3p orbitals of the Al3 atom overlap with the 4d (3d) orbitals of the impurity atom Nb (Ti, V) from -12 eV to -5 eV, which is consistent with strong bonding interactions between

the impurity atom and neighbouring host atoms. The above results are consistent with the analyses on the interatomic energy and charge density.

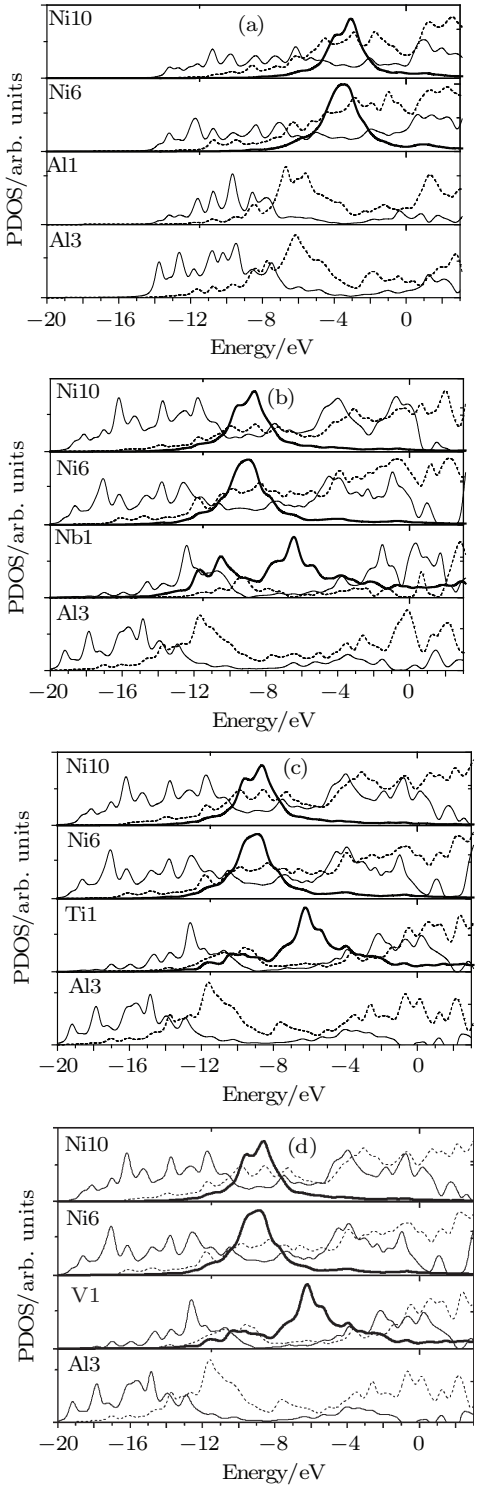


Fig. 4. The PDOS curves for impurities and neighbouring host atoms in (a) the clean DC; (b) the Nb-doped DC; (c) the Ti-doped DC; (d) the V-doped DC. The thick solid lines, thin solid lines, and dashed lines denote d, s, and p electronic states, respectively. The Fermi level shifts toward zero. The Arabic numbers correspond to those in Fig. 1.

In general, the behaviour of refractory impurities (such as Nb, Ti, and V) and their influence on the host atoms have similarities. The interactions between impurity and host atoms in the dislocation core are enhanced by the hybridization between impurity 4d5s (3d4s) and Ni 3d4s4p orbitals, as well as the 3s3p orbitals of the host Al atom.

4. Conclusions

In this work, we studied the alloying effect of refractory elements such as Nb, Ti, and V in the [100] (010) edge DC of NiAl using the first-principles DMol method and DVM. Two geometrical models are considered for the calculation of the impurity segregation energy in the DC. The results of segregation energy shows that the impurity Nb (Ti, V) prefers to occupy the Al site in the centre-Al DC. The introduction of an impure atom into the DC significantly affects energetics as well as the electronic structure of the DC. The calculation results of interatomic energy show that the bond strength between the host atoms increases in each of the doping impurity systems. Especially, the interactions between the impurity atom and its nearest-neighbouring host atoms (Ni6, Ni10) are much stronger than those between the Al1 atom and its corresponding host atoms in the clean DC. In addition, the charge distribution and PDOS results indicate that some charge accumulations appear between the impurity atom and nearest-neighbouring Ni atoms, and the strong bonds formed between the impurity atom and neighbouring host atoms due mainly to the hybridization of the 4d5s (3d4s) orbitals of the impurity atom Nb (Ti and V) and the 3d4s4p orbitals of host Ni atoms. The impurity–dislocation interaction should give an effective contribution to strengthen the NiAl alloy. These results provide a basis for understanding the physical factor and microscopic mechanisms of solid-solution hardening upon alloying in a NiAl alloy.

References

[1] Peter L and Raimund P 2009 *Intermetallics* **17** 675
[2] Misra A and Gibala R 2000 *Intermetallics* **8** 1025
[3] Misra A, Wu Z L, Kush M T and Gibala R 1997 *Mater. Sci. Eng.* A **239–240** 75
[4] Ramassundaram P, Bowman R and Soboyejo W 1998 *Mater. Sci. Eng.* A **248** 132

[5] Medvedeva N I, Gornostyrev Yu N, Kontsevoi O Yu and Freeman A J 2004 *Acta Materialia* **52** 675

[6] Ball A and Smallman R E 1966 *Acta Metall.* **14** 1349

[7] Takasugi T, Kishino J and Hanada S 1993 *Acta Metall. Mater.* **41** 1009

[8] Hu J and Lin D L 2008 *Mater. Sci. Eng.* A **490** 157

[9] Yang C 2006 *Int. J. Mech. Sci.* **48** 950

[10] Ghosh B and Crimp M A 1997 *Mater. Sci. Eng.* A **239**–**240** 142

[11] Ebrahimi F and Shrivastava S 1998 *Acta Mater.* **46** 1493

[12] Pollock T M, Lu D C, Shi X and Eow K 2001 *Mater. Sci. Eng.* A **317** 241

[13] Fu C L and Zou J 1996 *Acta Mater.* **44** 1471

[14] Kontsevoi O Yu, Gornostyrev Yu N, Freeman A J, Katsnelson M I and Trefilov A V 2001 *Philos. Mag. Lett.* **81** 455

[15] Chen L Q and Yu T 2011 *Sci. Chin.: Phys. Mech. & Astron.* **54** 815

[16] Miracle D B 1993 *Acta Metall. Mater.* **41** 649

[17] Wang Y L, Jones I P, and Smallman R E 2006 *Intermetallics* **14** 800

[18] Delley B 1991 *J. Chem. Phys.* **94** 7245

[19] Delley B 1990 *J. Chem. Phys.* **92** 508

[20] Ellis D E and Painter G S 1970 *Phys. Rev.* B **2** 2887

[21] Guenzburger D and Ellis D E 1992 *Phys. Rev.* B **46** 285

[22] Voter A F and Chen S P 1987 *High Temperature Ordered Intermetallic Alloys*, eds by Siegel R W, Weertman J R and Sundan R *MRS Symposia Proceeding* No. 82 (Pittsburgh: Materials Research Society) p. 175

[23] Zhang H, Wu H Y, Chen Y Y and Cheng X L 2006 *Chin. Phys.* **15** 428

[24] Zhu T and Wang C Y 2006 *Chin. Phys.* **15** 2089

[25] Chen L Q, Wang C Y and Yu T 2008 *Chin. Phys.* B **17** 662

[26] Chen L Q, Wang C Y and Yu T 2006 *J. Appl. Phys.* **100** 023715

[27] Wang S Y, Wang C Y, Sun J H, Duan W H and Zhao D L 2001 *Phys. Rev.* B **65** 035101

[28] von Barth U and Hedin L 1972 *J. Phys.* C **5** 1629

[29] Yan J A, Wang C Y, Duan W H and Wang S Y 2004 *Phys. Rev.* B **69** 214110

[30] Allaverdova N V, Portnoy V K, Kucherenko L A, Ruban A V and Bogdanov V I 1988 *J. Less-Common Metals* **141** 191

[31] Duncan A J, Kaufman M J, Liu C T and Miller M K 1994 *Appl. Surf. Sci.* **76-77** 155

[32] Bozzolo G, Noebe R D and Honecy F 2000 *Intermetallics* **8** 7

[33] Wang C Y and Zhao D L 1994 *Mater. Res. Soc. Symp. Proc.* **318** 571

[34] Wang C Y 1995 *Defect Diffus. Forum* **125**–**126** 79