Rare Metal Materials and Engineering
Volume 47, Issue 9, September 2018
Online English edition of the Chinese language journal

Cite this article as: Rare Metal Materials and Engineering, 2018, 47(9): 2687-2692.

ARTICLE

Effects of Point Defects on Properties of B2 NiAl: A First-principles Study

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Abstract: The basic properties, heats of formation, energies of formation, equilibrium concentration of point defects, elastic properties, and electronic structures for point defect structures of B2-NiAl crystal were analyzed by the density functional theory. Compared with B2-NiAl and other B2 intermetallic compounds, purity NiAl has better ductility and bonding strength. According to the calculated heats of formation, energies of formation, and equilibrium concentration of point defects, the Ni antisite and Ni vacancy are primary defects in B2-NiAl crystal. The calculated G/B_0 and Cauchy pressure parameters C_{12}–C_{44} values confirm that Ni vacancy, Ni antisite, and Al antisite can promote the brittleness of B2-NiAl, in which Ni vacancy is the primary defect, while Al vacancy with a low concentration can improve ductility of B2-NiAl. The density of state confirms that B2-NiAl intermetallic compounds are conductors, and point defects can promote the stability of the system expect Ni antisite defect.

Key words: NiAl alloy; point defects; elastic properties; first-principles

The intermetallic compound NiAl is one of the most promising high-temperature materials because of its high melting temperature, excellent oxidation resistance, high thermal conductivity and low density. But its poor strength at high-temperature, fracture toughness and ductility at room temperature restrict its commercial applications[1-5]. Particularly, improving the properties of ductility has aroused widespread concern in both theory and experiment.

Some efforts have been made in order to improve ductility of NiAl at room temperature by record effects of macroalloying, microalloying, and reinforcing ductile second phase [6-8]. Although these efforts have been made, the brittleness is still a major problem for the application of NiAl at room temperature. Pure NiAl is ductile material, which has been demonstrated by many investigations [9, 10]. However, NiAl has a poor ductility at room temperature. It is generally believed that trace (PPM) impurities can lead to the change of mechanical properties of materials [11]. One of the uncontrollable factors of impurity plays an important role in the mechanical properties of NiAl. There are many types of impurities consisting of boron, oxygen, nitrogen, carbon, phosphorus, silicon, sulfur and point defects in NiAl[12]. A minor impurity such as point defects has been taken as one possible cause for the room temperature brittleness of the intermetallics. Many physical and mechanical properties are dramatically related to the presence of point defects[13, 14]. G. V. Sinko et al. [15] have studied NiAl microalloyed with Y, Sc, Nd and La by first-principles, and found that the above four rare earth microalloying elements could improve the ductility of NiAl, and Ni8Al7La was more ductile than the NiAl, Ni8Al7Sc showed the largest hardness among them. C. Jiang[16] have studied the prioritized lattice site of Pt in B2 NiAl by the first-principles combined with experiments, considered the influence of point defects which contain Al antisite, Al vacancy, Ni antisite and Ni vacancy on properties of NiAl alloys, and found that the Ni vacancy and Ni antisite are the primary point defects. Xuelan Hu et al. [17] has record the influence of O impurity on mechanical properties and structure of NiAl intermetallics by first-principles,

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Received date: September 22, 2017
Foundation item: National Natural Science Foundation of China (51574176); Program for the Top Young Academic Leaders of Higher Learning Institutions of Shanxi (TYAL) (143020142-S); Major Research & Development Plan of Shanxi Province (International Cooperation Project) (201603D421028)
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and found that O atom can either go into the tetrahedron interstitial site or replace Ni atom; it depends on the surrounding environment and leads to decrease in the ductility and increase in the brittleness of NiAl. Lv Chen[18] considered the influence of point defects on mechanical properties of NiAl when Fe was added into NiAl, and found that the ductility of NiAl was decreased by the Ni vacancy and Ni antisite.

The point defects in NiAl have been investigated in certain areas, yet a comprehensive study of influence of point defects on properties of NiAl is still poor in the field of literature. In order to make up this kind of vacancy, the following heats of formation, basic properties, energies of formation, equilibrium concentration of point defects, elastic properties and electronic structures for point defect structures in B2-NiAl crystal will be explored with first-principle methods in this study.

1 Crystal Structure and Calculation Details

Density functional theory (DFT) with ultrasoft pseudopotentials[19] is employed in the Cambridge serial total energy package (CASTEP), which uses plane-wave pseudopotential to display first-principles quantum mechanics calculations. Perdew et al described the Generalized gradient approximation (GGA). It was applied as exchange-correlation functional for all elements in our models[20]. This program was used to record the basic properties, heats of formation, energies of formation, equilibrium concentration of point defects, elastic properties, and electronic structures of the Ni8Al8 (2×2×2) supercell with addition of Al antisite (Ni7Al9), Al vacancy (Ni8Al7), Ni antisite (Ni9Al7), and Ni vacancy (Ni7Al8).

The unit cell of NiAl was established with the space group PM-3M and the lattice constant of 0.289 nm, which includes one Al atom at (0, 0, 0) and one Ni atom at (1/2, 1/2, 1/2), and is shown in Fig.1a. The values of kinetic energy cutoff (E_{cut}) were set to 400 eV and the k-point to 4×4×4 with a regular Monkhorst-Pack scheme. In the process of calculation of self-consistent field (SCF), the Pulay scheme of density mixing[21] was used. The electronic structure and the elastic constants were calculated by cell optimization with a convergence tolerance of energy of 4.0×10^{-6} eV/atom, a maximum displacement of 4.0×10^{-5} nm and a maximum force of 0.1 eV/nm, respectively. A supercell model of NiAl with point defects, which contains 16 atoms is shown in Fig.1b.

2 Results and Discussion

2.1 Basic properties of B2-NiAl crystal

The lattice parameter optimized in this paper is 0.2899 nm, which coincides with other theoretical data 0.2870 nm [18] and the experimental data 0.2886 nm[22]. The calculated elastic constants as shown in Table 1 also fit perfectly other calculation data[17,18] and experimental data[23,24], proving that the proposed computational methodology is perfect for our current purpose and our geometry optimizations results are reliable.

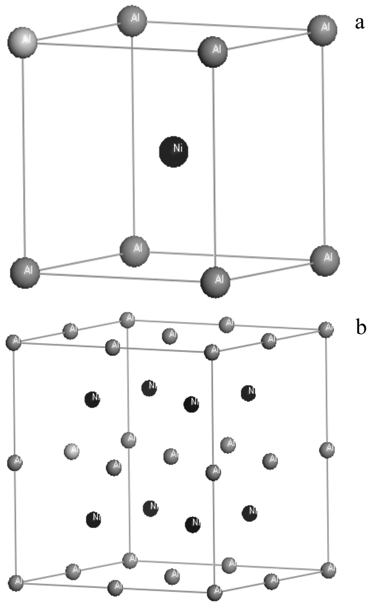

Fig.1 Models of calculation: (a) crystal structure of B2-NiAl and (b) Ni8Al8 supercell (2×2×2)

It has been recently found that Cauchy (C_{12}–C_{44}) is very significant to the mechanical properties of materials. The Cauchy pressure of metallic bond is positive. The larger the value, the stronger the ductility. In contrast, Cauchy pressure of covalent bond is negative. The larger the value, the stronger the brittleness[25]. The calculated Cauchy (C_{12}–C_{44}) of B2-NiAl and several kinds of B2 intermetallic compounds are shown in Table 2. In our calculation, the interaction between atoms of NiAl and RuAl are of metallic bond, since the Cauchy pressure value is positive. However, the interaction between atoms of ScAl, FeAl and CoAl are of covalent bond, because its Cauchy pressure value is negative. In a word, pure NiAl has the best ductility compared with other B2 intermetallic compounds, since its Cauchy pressure value is the highest.

Bonding strength of material is indirectly characterized by the melting temperature of alloy, which can be calculated by the following expression:

$$T_{\mathrm{m}}=[533\ \mathrm{K}+(5.91\ \mathrm{K/GPa})C_{11}]\pm300\ \mathrm{K} \tag{1}$$

The calculated melting temperature of B2 intermetallic compounds is shown in Table 2, which coincides well with the previous calculation results and available experimental data. Comparing the values, we find that our calculation value is higher than experimental data. There are many reasons accounting for this point: firstly, our calculated C_{11} value temperature was at 0 K, while experimental data was measured at higher temperature; secondly, B2 NiAl considered here was pure substance, which is not involved in the defects in the crystal. Comparing the melting temperature values of B2 NiAl and other B2 intermetallic compounds, we can find the melting temperature of B2 NiAl is relatively lower than those of others, which further proves that the bonding strength of B2 NiAl is relatively lower as well.

Table 1 Comparison of elastic constants calculated in this work with precious other calculation (Cal.) and experimental (Exp.) values for pure B2-NiAl crystal

Reference	C_{11}/GPa	C_{12}/GPa	C_{44}/GPa	B_0/GPa	G/GPa	v	E/GPa
This work	167	152	98	157	62	0.323	164
Cal.[18]	161	148	97	152	61	0.319	161
Cal.[17]	172	146	100	-	-	-	-
Exp.[24]	211	143	112	-	-	-	-
Exp.[23]	199	137	116	158	-	-	-

Table 2 Elastic constants, Cauchy pressure parameter (C_{12}–C_{44}) and melting temperature T_m of B2-NiAl and other similar B2 intermetallic compounds

Parameter	CoAl[25]	FeAl[25]	ScAl[25]	RuAl[25]	NiAl
C_{11}/GPa	313	272	96	322	167
C_{12}/GPa	105	140	62	143	152
C_{44}/GPa	135	142	92	121	98
C_{12}-C_{44}/GPa	-30	–2	–30	22	54
T_m(Cal.)/K	2403	2161	1120	2456	1539
T_m (Exp.)/K[26]	1921	1583	-	2193	1911

2.2 Heats of formation

Heats of formation (H_{form}) of point defect structures in B2-NiAl per atom with different structures are calculated by the following formula [27]:

$$H_{form} = \frac{1}{x+y}(E_{tot} - xE_{solid}^{Ni} - yE_{solid}^{Al}) \tag{2}$$

Where E_{tot} represents the total energy of supercell used in the current calculation, x and y represent the numbers of Ni and Al atoms, respectively. E_{solid}^{Ni} and E_{solid}^{Al} represent the energies of per fcc-Al and fcc-Ni atoms in the solid states, respectively. Using the same code as primitive cell, the calculated energy values of Ni and Al atoms are −1354.382 and −56.441 eV, respectively. The total energies of these point defects in B2-NiAl are listed in Table 3, and the H_{form} calculated from Eq.(2) are also shown in Fig.2.

Based on the data from Fig.2, H_{form} of Ni_8Al_8 is −66.47 kJ/mol·atom, approximating the corresponding calculation value of −71.3 kJ/mol·atom[18], which shows good agreement with the corresponding experimental value −72.0 kJ/mol·atom[27]. Further analysis reveals that the heats of formation are all negative, which means that these point defects can exist stably. The absolute H_{form} of Ni_7Al_8 (Vac.Ni) and Ni_9A_{l7} (anti.Ni) are all higher than those of others, which can prove that Ni antisite and Ni vacancy are the main point defects in B2-NiAl. This is also in good agreement with other calculation analysis[18].

2.3 Formation energy and equilibrium concentration of point defects

Energies of formation of point defect structures in B2-NiAl per atom with different type structures are calculated by the following formula [28]:

$$E_A^V = [E(A_7B_8) - E(A_8B_8)] + E(A) \tag{3}$$

$$E_A^B = [E(A_9B_7) - E(A_8B_8)] + [E(B) - E(A)] \tag{4}$$

Where A, B are Ni atom and Al atom, respectively. $E(A_7B_8)$,

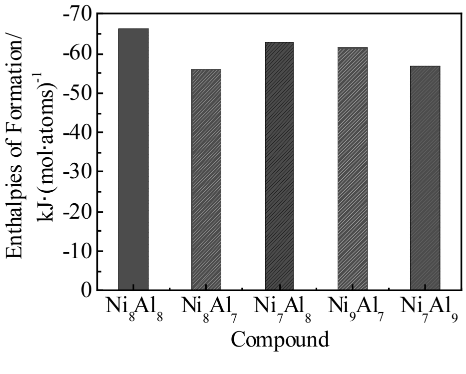

Fig.2 Calculated heats of formation for point defect structures of B2-NiAl crystal

Table 3 Total energies, formation energy and equilibrium concentration of point defects in B2-NiAl crystal

Compound	Total energies/eV	Energies of formation/eV	Equilibrium concentration of Point defects
Ni_8Al_8	−11297.62	-	-
Ni_8Al_7(Vac.Al)	−11238.85	2.325	2.7×10^{-40}
Ni_7Al_8(Vac.Ni)	−9941.95	1.281	1.6×10^{-22}
Ni_9Al_7(anti.Ni)	−12594.71	0.8503	3.4×10^{-15}
Ni_7Al_9(anti.Al)	−9998.06	1.613	3.6×10^{-28}

$E(A_8B_8)$ and $E(A_9B_7)$ are the total energies of the vacancy crystal, perfect crystal and antisite crystal, respectively. $E(A)$ and $E(B)$ are the average energy of atom in the solid state. Formation energy of these point defects in B2-NiAl crystal were calculated with Eq. (3) and Eq. (4) and are shown in Table 3.

According to Table 3, we can find that the energies of formation calculated values of Ni vacancy and Ni antisite are lower than that of Al atoms in B2-NiAl, which proves that Ni vacancy and Ni antisite are more easy to form.

The equilibrium concentration of point defects at T is calculated with the following equation[29]:

$$C_e = A\exp(\frac{-E_V}{kT}) \tag{5}$$

Where C_e is the equilibrium concentration of point defects, A is a material constant, and is often taken to 1. T is the thermodynamic temperature of systems. k is the Boltzmann constant, and generally is 8.62×10^{-5} eV/K or 1.38×10^{-23} J/K. E_V is the energy of formation. The equilibrium concentration of point defects in B2-NiAl crystal at room temperature (296.15 K) calculated from Eq. (5) is shown in Table 3.

According to Table 3, we can find the calculated equilibrium concentration of point defects at room temperature is very low, and the Ni vacancy and Ni antisite are primary defect structures in B2-NiAl crystal.

2.4 Elastic properties

As everyone knows that the elastic modulus of materials are usually used to assess certain macroscopic mechanical properties[30, 31], such as strength, hardness and ductility, which are related to the microscopic elastic constants. However, it is difficult to get elastic constants accurately for the precision of testing facilities and defects in materials. Here, it is a prior consideration that theoretical calculation is based on first principles.

The independent elastic constants in the cubic phase are C_{11}, C_{12}, and C_{44}, from which we can receive the bulk modulus B_0, shear modulus G, Poisson' ratio ν and Young's modulus E[32]:

$$B_0=(C_{11}+2C_{12})/3 \tag{6}$$

$$G=(3C_{44}+C_{11}-C_{12})/5 \tag{7}$$

$$v=(E-2G)/2G \tag{8}$$

$$E=9B_0G/(3B_0+G) \tag{9}$$

The elastic constants C_{11}, C_{12}, C_{44}, bulk modulus B_0, shear modulus G, Poisson' ratio v and Young's modulus E are shown in Table 4. The data of Ni_8Al_8, Ni_7Al_8 (VacNi), and Ni_9Al_7 (antiNi), reveals that our calculated results are coincide with other experimental and theoretical analysis[15,17,18,33,34], with a gap within 10%. Many reasons can account for this point: firstly, the materials of defects were ignored in their theoretical calculations; secondly, the effects of anisotropy on the elastic properties were neglected in experimental investigation.

The mechanical stability criteria in cubic crystal are: $B_0>0$, $C_{11}-C_{12}>0$, $C_{44}>0$[35,36]. The elastic constants of calculated prove that all point defect structures in B2-NiAl crystal are stable.

According to Fig.3, we can find the calculated G/B_0 and Cauchy pressure parameters $C_{12}-C_{44}$ values are in agreement with other results of experimental and calculation for Ni_8Al_8, Ni_7Al_8, and Ni_9Al_7. In as early as 1954, Pugh concluded that G/B_0 reflects the ductility of the pure metals: the larger the G/B_0, the more ductile the metal, which is also applicable to the intermetallic compounds. The critical value of G/B_0 which separates ductility and brittleness is fixed at about 0.50[37]. The calculated G/B_0 values of Ni_8Al_8, Ni_8Al_7 (VacAl), Ni_7Al_8 (VacNi), Ni_9Al_7 (antiNi), and Ni_7Al_9 (antiAl) are 0.476, 0.417, 0.647, 0.492, and 0.494, respectively, which are shown in Fig.3a. So Ni_8Al_8, Ni_8Al_7 (VacAl), Ni_9Al_7 (antiNi), and Ni_7Al_9 (antiAl) compounds are considered as ductile materials, yet Ni_7Al_8 (VacNi) is a brittle material. It further proves that the Ni vacancy, Ni antisite and Al antisite can promote brittleness of B2-NiAl, and in which the Ni vacancy is the primary defect, while Al vacancy with a low concentration can improve ductility of B2-NiAl. Cauchy pressure parameters $C_{12}-C_{44}$ has been also taken as a criterion for ductile and brittle material. If the value is positive, the crystal is ductile; otherwise, the crystal is brittle. In Fig.3b, the same conclusions can be obtained with G/B_0 for B2-NiAl. Therefore, our calculation results

Table 4 Calculated and experimental elastic constants for point defect structures in B2-NiAl crystal(GPa)

Compound	C_{11}	C_{12}	C_{44}	B_0	G	v	E	Reference
Ni_8Al_8	174	149	117	157.5	75	0.29	194	This work
	199	137	116	158.7	82	0.27	209	Exp.[33]
	205	135	117	158.5	84	0.27	214	Exp.[34]
	173	149	117	157.4	75	0.29	194	Cal.[15]
	208	132	112	157.8	82	0.27	211	Cal.[17]
Ni_8Al_7(VacAl)	192	134	86	153.3	64	0.32	169	This work
Ni_7Al_8(VacNi)	217	105	116	142.3	92	0.23	227	This work
	209	107	122	141.0	94	0.26	238	Cal.[18]
Ni_9Al_7(antiNi)	212	144	114	166.7	82	0.28	211	This work
	214	142	117	166.0	85	0.28	218	Cal.[18]
Ni_7Al_9(antiAl)	141	118	95	125.5	62	0.29	160	This work

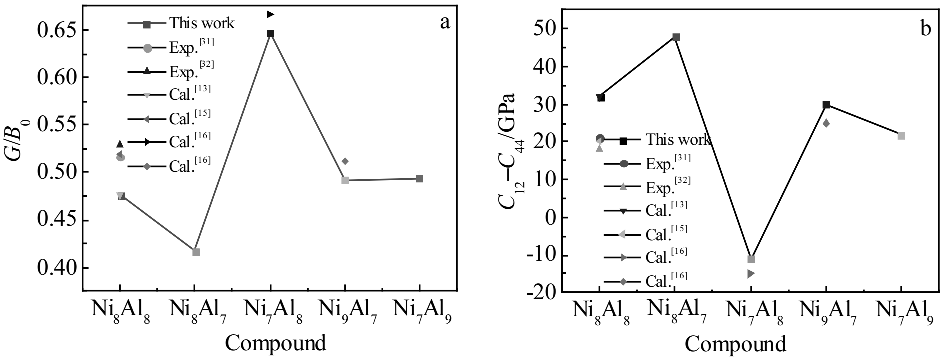

Fig.3 Calculated G/B_0 (a) and Cauchy pressure parameters C_{12}–C_{44} values (b) compared with values of experimental and other theoretical for point defect structures in B2-NiAl crystal

show that the pure B2-NiAl has a fine ductility, yet B2-NiAl has a poor ductility at room temperature, which may be attributed to the reason that a small amount of point defects exist in B2-NiAl at room temperature.

2.5 Density of state

Finally, we calculated the density of state for point defect structures in B2-NiAl crystal with their optimized crystal lattices. The results are shown in Fig.4. Density of state at Fermi level can be taken as a criterion for stability and conductor, the smaller the value of density of state at Fermi level, the more stable the system. The intermetallic compound can be a semiconductor or an insulator when its density of state at Fermi level is zero; otherwise, it is a conductor. As shown in Fig.4, the values of density of state at Fermi level for Ni_8Al_8, Ni_8Al_7 (VacAl), Ni_7Al_8 (VacNi), Ni_9Al_7 (antiNi), and Ni_7Al_9 (antiAl) are 8.1011, 7.1683, 7.4463, 8.2671, and 6.2283 eV, respectively, revealing the B2-NiAl intermetallic compounds are conductors, and the point defects can promote the stability of the B2-NiAl intermetallic compounds expect Ni antisite defect.

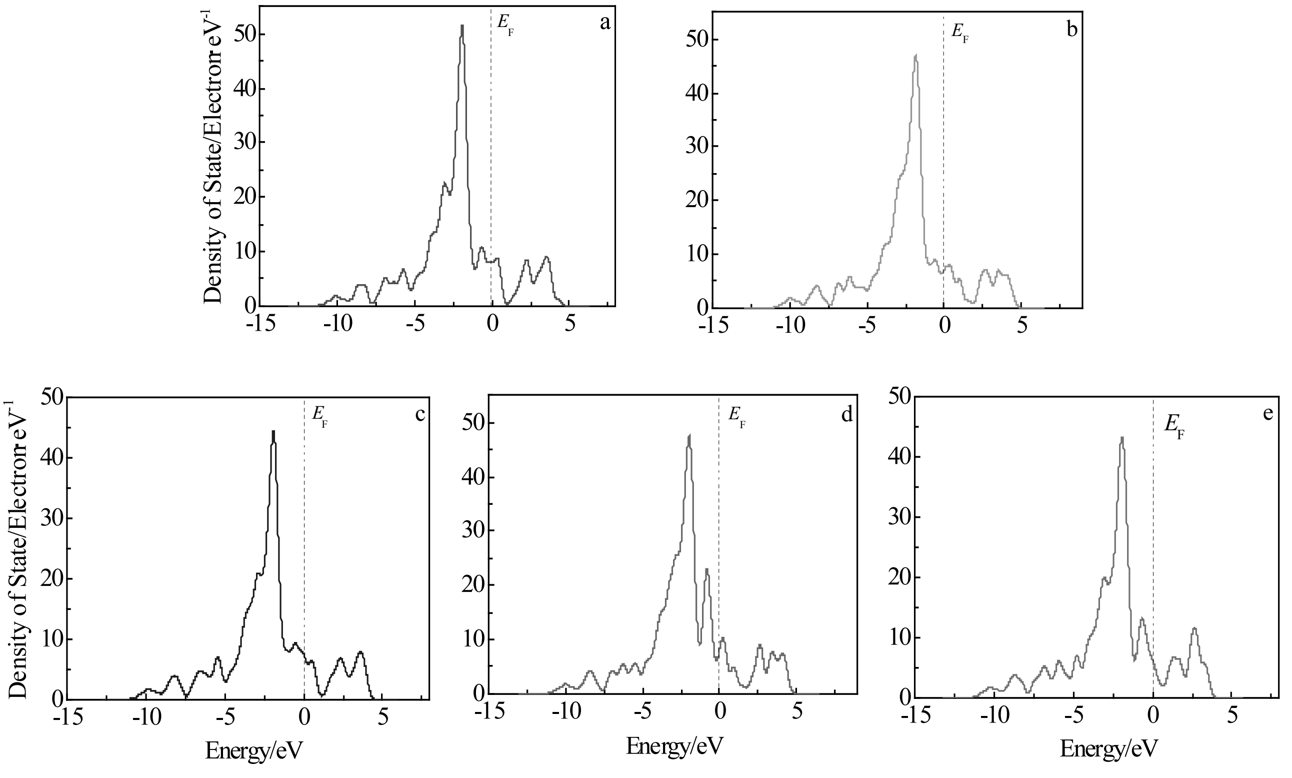

Fig.4 Calculated density of state for point defect structures in B2-NiAl crystal: (a) Ni_8Al_8, (b) Ni_8Al_7, (c) Ni_7Al_8, (d) Ni_9Al_7, and (e) Ni_7Al_9

3 Conclusions

1) Comparing the B2-NiAl with other B2 intermetallic compounds, pure NiAl has better ductility and stronger bonding strength than others.

2) With the calculated heat of formation, energy of formation and equilibrium concentration of point defects, the Ni antisite and Ni vacancy are primary defect structures in B2-NiAl crystal.

3) The calculated G/B_0 and Cauchy pressure parameters C_{12}–C_{44} values confirm that Ni vacancy, Ni antisite, and Al antisite can promote brittleness of B2-NiAl, in the Ni vacancy is the primary defect, while Al vacancy with a low concentration can improve ductility of B2-NiAl.

4) The calculated density of state shows that B2-NiAl intermetallic compounds are conductors, and point defects can promote their stability expect Ni antisite defects.

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第一性原理研究点缺陷对 B2 结构 NiAl 合金性能的影响

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摘　要：采用基于密度泛函理论的第一性原理计算分析了含点缺陷结构 NiAl 晶胞的形成热、形成能、点缺陷平衡浓度、力学性能、电子结构等。将 NiAl 与其他 B2 结构的金属间化合物进行对比，发现 NiAl 拥有更好的塑性和成键强度。根据形成热、形成能和点缺陷平衡浓度的计算结果，发现 Ni 反位和空位缺陷是 NiAl 晶胞结构中主要的点缺陷。通过 Pugh（G/B_0）和 Cauchy（C_{12}–C_{44}）准则预测出 Ni 空位和反位缺陷、Al 反位缺陷能够提升 NiAl 合金的脆性，其中 Ni 空位缺陷作用最明显；而 Al 空位缺陷能够改善 NiAl 合金的塑性，但在 NiAl 合金中的浓度很低。态密度计算结果发现 NiAl 合金具有良好的导电性能，Ni 空位缺陷、Al 空位和反位缺陷能够提升 NiAl 合金的稳定性。

关键词：NiAl 合金；点缺陷；力学性能；第一性原理

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