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ω -phase formation in NiAl and Ni₂Al alloys

M Sanati^{1,2,3}, R C Albers² and F J Pinski³

¹ National Renewable Energy Laboratory, Golden, CO 80401, USA

² Theoretical Division, Los Alamos National Laboratory, Los Alamos NM 87545, USA

³ Department of Physics, University of Cincinnati, Cincinnati, OH 45221, USA

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Abstract

The phase stability of bcc-like NiAl and Ni₂Al with respect to phase transformations into the ω phase is examined by first-principles, full-potential, linear muffin-tin orbital method (FPLMTO), band-structure calculations. In agreement with experiment we find that bcc-like NiAl is stable, whereas Ni₂Al is unstable. We have also performed some calculations in slightly disordered phases, and find that the disordering tends to inhibit the transformation. This supports the suggestion that a combined displacive/ordering transformation mechanism is involved in the phase transformations of the Ni₂Al system. Calculated lattice parameters and the degree of internal shuffling of atoms for the ordered Ni₂Al phase were found to be in excellent agreement with the experiment.

1. Introduction

Alloys of Ni and Al have long been important candidates for strong, light-weight, high-temperature, structural materials. At high temperatures these materials tend to form ordered bcc-like alloys for a large range of stoichiometry around 50% Al and 50% Ni. However, similar to many bcc-like alloys, they are often susceptible to transitions into an ω -type crystal structure (which collapses every second and third plane of the bcc structure along the [111] direction). In this paper we examine the stability of the bcc-like phases of these alloys both on stoichiometry as well as on the Ni-rich side of stoichiometry (at the NiAl and Ni₂Al stoichiometries) with respect to a transition to an ω -like phase. We also attempt to do some calculations to elucidate the possible effects of disorder on this stability.

Systems of Ni and Al tend to form strong partially covalently bonded intermetallic compounds. Because of the strong Ni–Al and Ni–Ni bonds, they tend to hold together quite well at very high temperatures (e.g., high melting points) and are therefore excellent candidates for structural materials that must operate at high temperatures (e.g., for turbine blades in aircraft). Their relatively low density and excellent oxidation resistance add to their attractiveness for these applications. Like many other strong materials, their chief drawback is their lack of ductility; they are often fairly brittle at lower temperatures. Because transitions to an ω structure tend to make the material even less ductile, it is important to understand the tendencies towards transitions into this structure. These materials also serve as a useful

paradigm for studying diffusionless phase transitions and the effects of disorder on such classes of phase transitions.

The Ni–Al alloy phase diagram is quite complicated. At either end (pure Ni or pure Al) the material is a close-packed cubic (fcc) metal. Near 50–50 atomic percent (NiAl), the alloys are an ordered CsCl (B2, bcc-like) phase. Across the whole concentration range (from zero to 100% Ni) a large number of stoichiometric phases form: Al, NiAl₃, Ni₂Al₃, NiAl, Ni₅Al₃, Ni₃Al, and Ni, with appropriate two-phase regions between many of the pure stoichiometries.

Near 50 atomic percent Ni (all percentages in this paper will refer to atomic percentages, not weight), there is a wide range of stoichiometry, ranging from just above 40% to a little below 70% Ni, depending on temperature, of an ordered cubic β_2 -phase (B2; CsCl-type; bcc-like structure). Below 50% Ni, the β_2 -phase tends to have vacancies on the Ni sites, and above 50% Ni, the excess Ni tends to sit on Al sites (of the CsCl structure).

Given this wide stoichiometry, the β_2 -phase tends to be surprisingly unstable on the Ni-rich side of stoichiometry. These tendencies in the β_2 -phase are present in its phonon dispersion curves; Shapiro *et al* [1], e.g., showed that the Ni-rich side of this system has two remarkable phonon anomalies. The first one is a softening of the (110) TA₂ branch at the Γ point. This phenomenon is now well known as a precursor of a martensitic transformation, and can be observed as a strain contrast, called ‘tweed’, in high resolution electron micrographs. The second phonon anomaly is characterized by a shallow dip at $q = \frac{1}{3}$ of the LA mode in (111) direction. This type of anomaly has been observed in systems exhibiting an ω -type transformation.

If the Ni–Al alloy is rapidly quenched near the Ni₂Al stoichiometry, it undergoes a martensitic phase transformation (displacive phase transformation) into multiply twinned 3R or 7M structures. Like many martensitic materials, a pre-transformational tweed-like structure is observed above the transformation temperature. If the quenched material is reheated at intermediate temperature, a new metastable structure, which is usually called the Ni₂Al structure, precipitates out. This precipitate has been identified by Muto *et al* [2, 3], who used high-resolution electron micrograph techniques to show that a one-dimensional partial ω -shuffle exists in the as-quenched β_2 phase (we use the term shuffle to mean moving some of the atoms inside the unit cell, while leaving the overall unit cell unchanged). This precipitate is metastable, since if it is annealed at higher temperatures or for longer periods of time, it usually decomposes into either β_2 , L1₂, or possibly Ni₅Al₃ structures.

The meta-stable phase of Ni₂Al was first found independently by Lasalmonie [4] and Reynaud [5]. Based on the results of electron diffraction patterns, Reynaud proposed a trigonal ($P\bar{3}m1$) ordered structure for this phase. It can best be understood by starting from a B2 (CsCl) structure of NiAl that is projected along the (111) direction (this corresponds to the $\langle 001 \rangle$ direction of the final trigonal structure). Reynaud’s structure results from replacing one of the Al (111) cubic planes of atoms with Ni atoms (see figure 1). Based on the similarity of diffraction patterns and an intensity anomaly of the super-lattice spots, Lasalmonie [6] suggested a similar structure, but with some collapse of the (111) stacking of planes. This is like the ω shuffle in bcc materials. The x-ray diffraction experiment [7] and phonon dispersion curve of the longitudinal cubic $\langle 111 \rangle$ branch [1] subsequently confirmed the existence of this ω -type structure inside the B2 matrix (note that the ω shuffle does not change the space group of the phase). Also, should the collapse of the planes go all the way to completion (the two planes collapse on top of each other), a B8₂ phase would be created (cf. figure 1(d)).

One key issue that has been controversial for these alloys is the relative roles of replacive (diffusional) and displacive transformations in determining the formation of the metastable structure. Muto *et al* [2, 3] in their recent high-resolution electron microscopy (HREM) method concluded that the formation of the Ni₂Al phase is a combined displacive/ordering

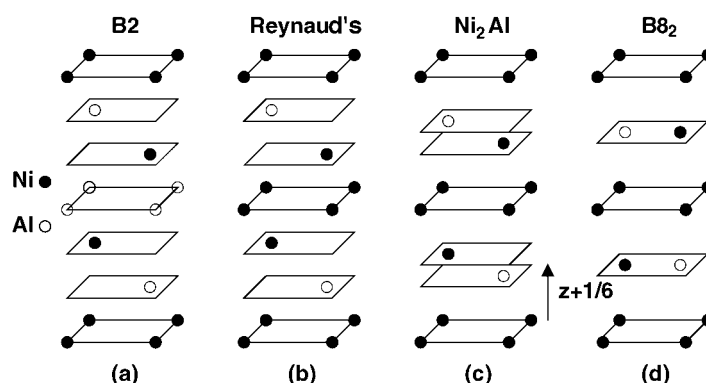


Figure 1. (a) stacking of the (111) planes of NiAl B2 structure, (b) Ni₂Al Reynaud's structure (equally spaced planes), (c) Ni₂Al structure with partial collapse of the planes, and (d) B8₂ structure (full collapse of two of the planes). The parameter z is indicated between parts (c) and (d) of the figure. It measures the movement of the first plane. When all planes are equidistant, $z = 0$, and the first plane is at a distance $1/6$ of c above the lowest plane. As the ω shuffle progresses to completion, this plane moves up by $1/12$ of c (the plane above it simultaneously moves down by $1/12$ of c). Although we have shown the ω collapse explicitly for Ni₂Al, the same collapse of planes could occur for NiAl as well, if it were to undergo an ω -phase transformation.

transformation and the amount of displacement (collapse of the two planes) was estimated to be between 20 and 50% of the full ω -type displacement.

In this paper we attempt to understand the formation and stability of ω -like phases with respect to bcc-like structures for ordered or partially ordered stoichiometric and Ni-rich Ni₂Al ordered alloys by means of first-principles, full-potential, linear muffin-tin orbital (FPLMTO) calculations. In agreement with experiment, we find that the CsCl structure is more stable than the ω -phase structures for NiAl, but this situation reverses itself for ordered Ni₂Al. Disordering the Ni₂Al (rearranging the atoms) has a tendency to reduce the ω -phase instability. In addition to the first-principles calculations, we have also tried to develop a crude understanding of these tendencies by fitting the band-structure results to simple radial pair-potential forces between the atoms; for the form of the pair potential we used a Lennard-Jones type [8]. Where the ω -like phase is stable, we have also calculated theoretical lattice parameters, and how much the second and third planes have collapsed.

2. Details of the band-structure calculations

We have used a full-potential linear muffin-tin orbital technique [9, 10, 11] in the calculations reported here. The calculations were all-electron, fully relativistic (with the spin-orbit coupling included at each variational step [12, 13]), and employed no shape approximation to the charge density or potential. The base geometry was a muffin-tin geometry with non-overlapping muffin-tin spheres; the basis function, charge density and potential were expanded in spherical harmonic series within the muffin-tins and in Fourier series in the interstitial. The basis set was comprised of augmented linear muffin-tin orbitals [12, 13]. The tails of the basis functions (the extension of the bases outside their parent spheres) were either Hankel or Neuman functions with non-zero kinetic energy. Four different tails for Ni-Al alloys were used. Spherical harmonic expansions were carried out through $l = 8$ for the bases, charge density and potential. For sampling the irreducible wedge of the Brillouin zone we used the special k -point method [14, 15, 16], with 32 and 58 k -points for unit cell with 6 and 12 atoms, respectively. For calculating the ground-state energies in addition to using the special k -point

technique we have, in order to speed up the convergence of the k -point sampling, associated each calculated eigenvalue with a Gaussian function having a width of about 5 mRyd. Finally, the calculations used the Hedin–Lundqvist exchange–correlation functional where gradient corrections to the exchange and correlation are included (GGA) [17].

3. Results

3.1. Band-structure calculations

We have calculated the theoretical zero-temperature crystal structure with the minimum energy for both NiAl and Ni₂Al. Because of the large number of degrees of freedom involved, we have searched for this structure by sequentially minimizing parameters expected to have the largest contribution to the overall energy. We began by constraining the c/a ratio to be $\sqrt{6}/2$ (theoretical value for the cubic structure), and then determined the lattice constant, a , through minimizing the energy. This procedure is roughly equivalent to determining the total energy as a function of the volume of the unit cell. After this was done, we then adjusted the c/a ratio by keeping the volume fixed. Finally, we allowed the collapse of the planes along the $(111)_{bcc}$ direction for the ω -type phase transformation.

Table 1. Calculated values for atomic parameters of NiAl and Ni₂Al systems. Experimental values taken from reference [7].

	NiAl (calc.)	NiAl (expt.)	Ni ₂ Al (calc.)	Ni ₂ Al (expt.)
a (Å)	2.889	2.886	2.850	2.857
c (Å)	3.535	3.535	3.505	3.505
z	0.0	0.0	0.025	0.02–0.04

Our results for the calculated atomic parameters for NiAl and Ni₂Al are in excellent agreement with experiment, as shown in table 1. Besides the a and c lattice constants we also calculated the total energy relative to z , the displacement of the planes (cf. the structure shown in figure 1(c) and 1(d); z is the displacement of the planes in units of c , where $z = 0$ corresponds to no collapse of the planes and $z = 1/12$ corresponds to a complete collapse of the two intermediate planes). The results of these calculations are shown in figure 2 for NiAl and Ni₂Al. For NiAl, we find that the lowest energy structure has z equal to zero (in agreement with experiment) and for Ni₂Al the value of z is between the experimental estimates. Based on the values of the other parameters and their good agreement with experimental values, our calculated value for the amount of plane displacement, z , for Ni₂Al is probably very reliable [18]. We find that the lowest energy structure for the Ni₂Al phase is of the incomplete ω -type (i.e., the planes are partially collapsed). It is possible that the high-resolution electron microscopy (HREM) measurements had difficulty in accurately detecting such a small value of the displacement of the atoms (z) [2, 3].

To confirm that our calculated structure for Ni₂Al is the correct stable one, we also calculated the total force on each atom in this structure and compared them with the forces within Reynaud’s (B2-type) structure. The results showed that the forces are fairly close to zero for the structure that corresponds to the minimum energy; the small differences from zero appear to be at the level of the numerical noise in the calculations.

Since NiAl is stable against ω -type transformations, no additional calculations were needed for this system. However, for the Ni₂Al system, we also did calculations for different

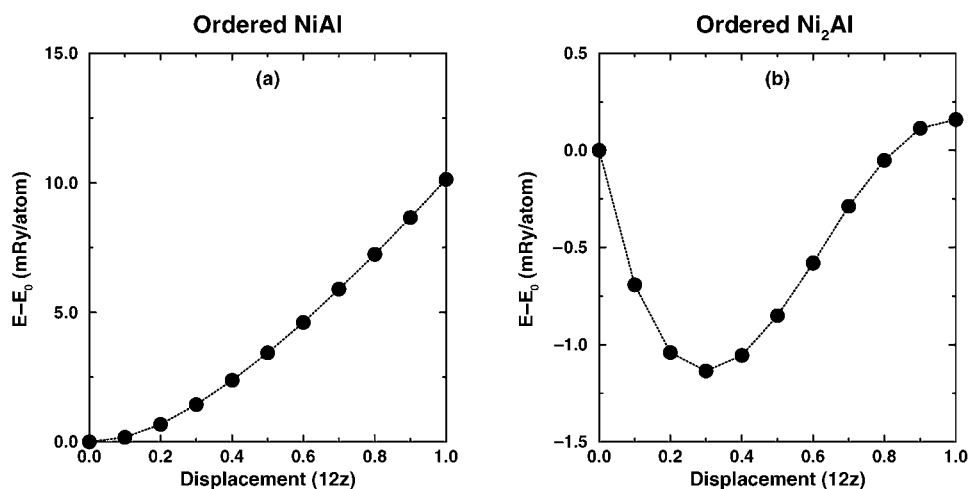


Figure 2. Total energy (full-potential FP-LMTO results) versus displacement, $12z$, for the ordered (a) NiAl and (b) Ni₂Al phase. When $12z = 1$, the ω shuffle is complete and two of the planes have completely collapsed upon each other. E_0 is the energy of the bcc-like structure for each system.

arrangements of the atoms inside the unit cell in order to examine the importance of atomic ordering to the stability of the crystal structure with respect to the ω transformation. Because of the potentially large number of possible arrangements, we attempted to use our experience with these systems (based on total energy calculations) to guess configurations which would be likely to have the lowest energies. We have found that such configurations are likely to have every Al atom surrounded by Ni atoms (to take advantage of the strong Ni–Al bonds; in contrast to the weak Al–Al bonds). In super-cells with six atoms per unit cell such a choice naturally leads to an ordered Reynaud’s structure. Hence, it is necessary to consider a bigger unit cell in order to study a disordered (rearranged) phase. Because of the rapidly increasing computational cost of larger super-cells, we restricted our consideration of disordered structures to those with 12 atoms per unit cell. Based on our experience, the most likely low-energy disordered arrangement of atoms in a 12-atom unit cell is that shown in figure 3, where we compare our disordered arrangement side by side with the ordered structure (clearly, what we call our disordered system is actually a rearrangement of the atoms in a larger supercell; it is the best we can do to mimic disorder within a periodic system, which is required by our band-structure method of calculation). For this configuration the bcc-like structure is stable against ω -type shuffles. In addition to the global collapse of planes in the supercell, we also tried some additional calculations where we collapsed only some of the planes (in one half of the supercell but not the other half) to further test stability of the structure. The result was the same: the bcc-like phase remained stable.

To check on the expected transition (diffusion) of atoms from a disordered to an ordered B2 phase of Ni₂Al we calculated the total energy of our disordered arrangement of atoms with the relevant ordered configuration; we found that the ordered configuration is lower in energy by -0.417 mRyd atom⁻¹ with respect to the disordered one.

These calculations suggest that the ordering of the different atoms in the Ni₂Al structure is critical in determining the stability of the structure with respect to the collapsing planes. This suggestion is consistent with the conventional wisdom that these transformations are driven by a Fermi-surface nesting and related phonon softening [19]. Any disorder will certainly tend to reduce such a nesting, and hence weaken the tendency towards the phase transformation. However, such tendencies can be difficult to quantify and the degree of nesting features in

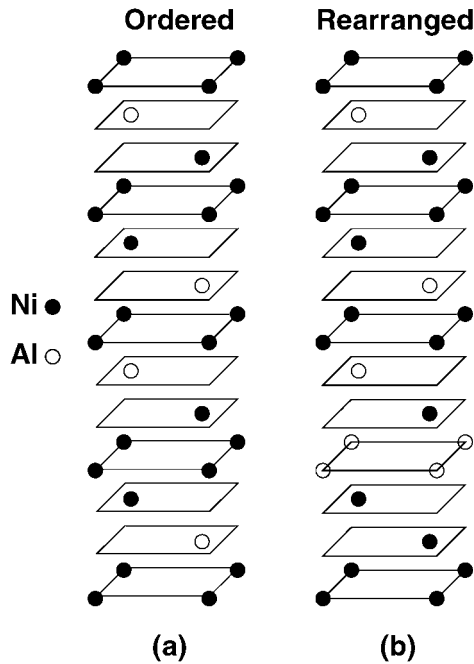


Figure 3. (a) Ordered Ni₂Al super-cell and (b) rearranged B2 structure.

various Fermi surface plots can depend somewhat on the eye of the beholder. For this reason we have not explored the expensive calculations (in the large unit cells used in this paper) needed to study the Fermi surface. We would be surprised if the conventional wisdom did not hold. In any event, the total energy differences are the quantitative measure of any such tendencies (the Fermi surface nesting just picks out one piece of the total energy), and we have very carefully calculated these differences in this paper. Our results unambiguously point to disorder inhibiting the transformation.

We have tried some simple pair-potential calculations that might have some heuristic value to experimentalists trying to guess trends. The first-principles results are the real results of this paper, and the pair-potentials should be viewed as only a crude parameterization of the first-principles results.

Given this caveat, as we will show below, from a pair-potential point of view, one can explain the transformation as being driven by unbalanced second-nearest-neighbour forces in the $\langle 111 \rangle$ direction on the Al atoms in the crystal, which cause the planes to collapse, when the Al atoms are at their normal (ordered) positions in the Reynaud structure. This driving force is removed when the Al atoms are replaced with Ni atoms. Hence, disordered structures where the Ni atoms occupy these sites tend to inhibit the ω -type collapse of the planes.

3.2. Pair-potential model

We have used a simple Lennard-Jones (LJ) potential in its general form [8] to model the band-structure results:

$$V(r) = D \left[\left(\frac{r_0}{r} \right)^m - \frac{m}{n} \left(\frac{r_0}{r} \right)^n \right].$$

Here, $V(r)$ is the potential energy between any two atoms separated by a distance r , r_0 is the distance where the potential is a minimum, and D , m , and n are potential parameters. Because the purpose of the fit was to qualitatively understand bonding tendencies, an approximate

quantitative agreement was deemed adequate and no attempt was made to fully optimize a pair potential (e.g., by using more elaborate functional forms or more parameters).

To calculate parameters we based all of our fits on the Ni₂Al structure. Because it has a partial ω -phase collapse rather than none, it is a more interesting case than NiAl. For the Al–Al and Ni–Ni bonds, we first used first-principles band-structure calculations to determine the energy of the ω -type displacement for structures with either all Al or all Ni atoms. We then fitted the appropriate Al or Ni potential to these energy curves to find the relevant potential single-element parameters; interactions up to third-nearest neighbours were included in the fit (cf. figure 4 to see how the bond lengths change for Ni₂Al as the ω collapse proceeds). Finally we used these Ni–Ni and Al–Al bonds (freezing these parameters) and fitted the energy curve obtained for the ordered Ni₂Al structure (figure 2) to obtain parameters for the Ni–Al bonds. Since all the structures of interest are variations of an underlying bcc lattice we did not change the lattice constants or crystal structure for calculating the Ni–Ni and Al–Al potential parameters. In this way we hoped to reduce other important effects such as directionality of the interactions (i.e., our fits are done for the geometry we are interested in; they may not work well for other crystal structures).

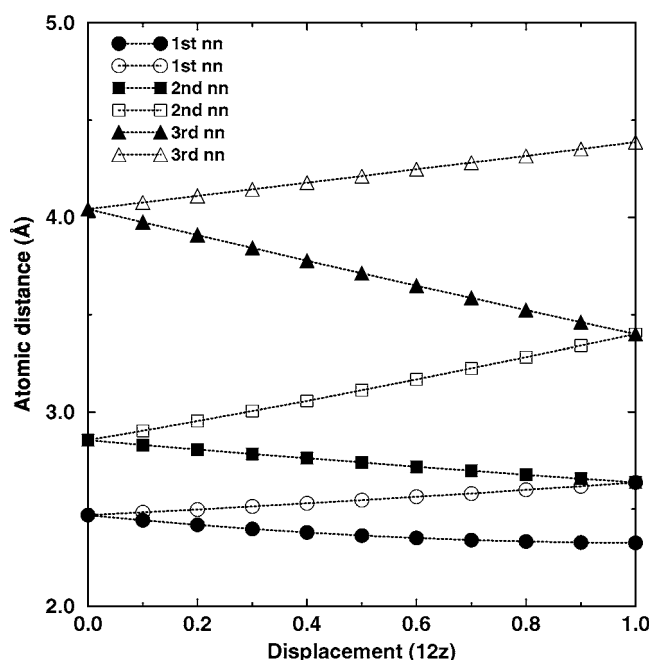


Figure 4. Nearest-neighbour distances (bond-lengths) for Ni₂Al as a function of $12z$ (splitting of bond lengths caused by the ω collapse).

Different potentials are shown in figure 5 and their related parameters are given in table 2. The results of the pair potential model for ordered and rearranged Ni₂Al systems and their comparison with *ab initio* calculations are shown in figures 6 and 7. Our pair potential model showed that the contributions of the third-nearest neighbours for the region of interest ($0 \leq 12z \leq 0.4$) is negligible, and one can restrict the search for the origin of stability or instability of each system up to only second-nearest-neighbour interactions. The NiAl results (cf., figure 6) are not as good as the Ni₂Al that we fitted to, but are nonetheless reasonably accurate. No attempt was made to further tune the parametrization.

Table 2. Parameters for the Lennard-Jones potential.

Bond	D (mRyd/atom)	m	n	r_0 (Å)
Ni–Al	1960.702	9.0651	8.6045	2.24089
Ni–Ni	2250.366	9.9315	9.4481	2.26010
Al–Al	672.938	9.4323	8.9600	2.42778

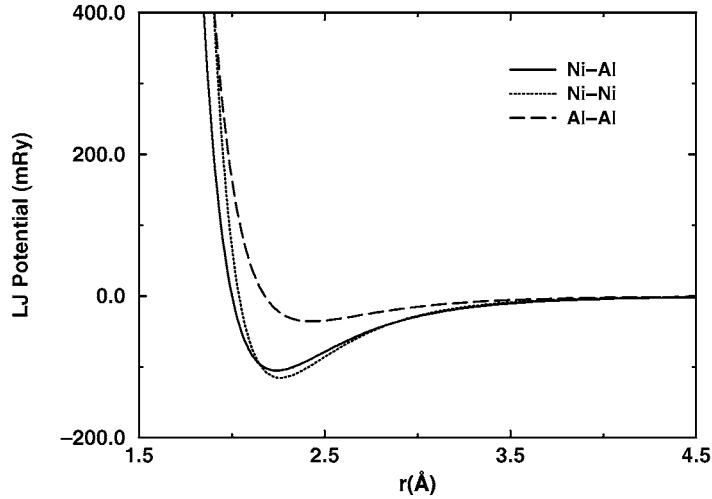
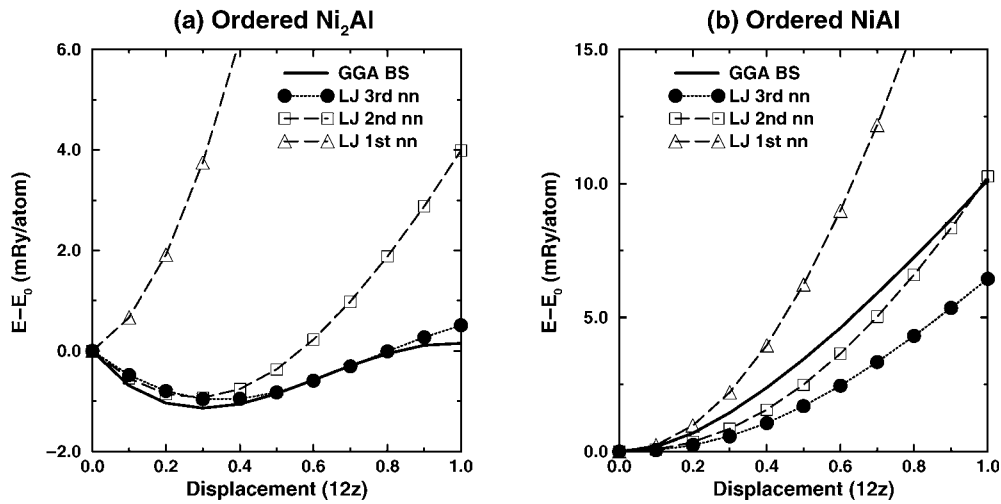
**Figure 5.** Lennard-Jones potential for different bonds.

Figure 6. Total energy as a function of displacement, $12z$, for ordered (a) Ni_2Al and (b) NiAl phase. When $12z = 1$, the ω shuffle is complete. The solid circles are the full-potential FP-LMTO results. The diamond and square points indicate results of the Lennard-Jones fit which add up to either second-nearest neighbours or including third-nearest neighbours in the total energy. Including the third-nearest neighbours allows a better total fit, but only second-nearest-neighbour interactions are needed to predict the presence or absence of ω -phase stability relative to a bcc-like structure.

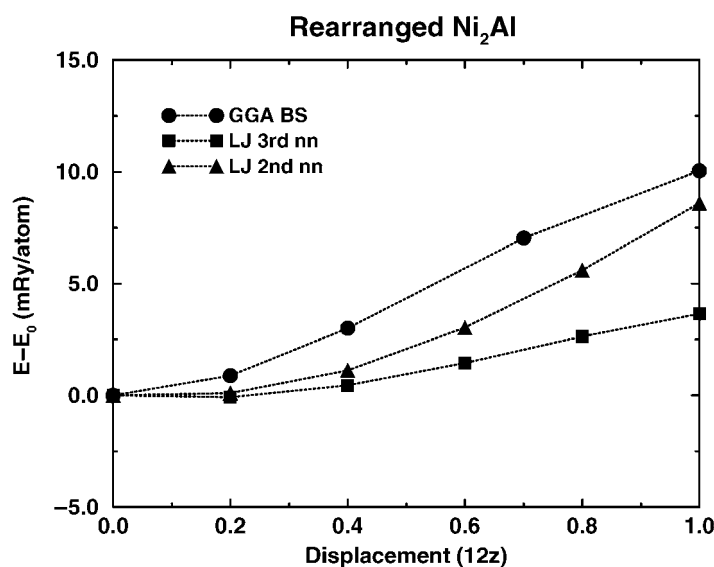


Figure 7. Comparison of total energy versus displacement, $12z$ for rearranged Ni₂Al phase, based on GGA and pair-potential results (up to second- and third-nearest neighbours).

4. Discussion

The pair potentials for each bond up to the second nearest shells are shown in figures 8 and 9 for ordered and rearranged Ni₂Al structures respectively. As figures 5, 8, and 9 show, Ni–Ni and Ni–Al bonds are comparable to each other and the Al–Al bond is much weaker. As the atoms shuffle during the transformation, specific pairs of atoms either approach or move away from each other. From figures 4 and 5 it is clear that the distances of minimum energy for the bonds (for any pair of atoms: Ni–Ni, Al–Al, or Ni–Al) is shorter than any of the nearest neighbour distances. Hence, any of the bond energies are always reduced when the atoms approach each other. However, by shuffling the atoms inside the unit cell, distances between some of the atoms increase, which increases the energy of the system. Therefore, stability or instability in each system depends on how these bonds balance each other, and the relative change in each bond's contribution to the energy with distance.

Experiment [7] has not found any ω -phase formation for the stoichiometric B2 NiAl system, which is clearly stable with respect to this type of transformation. The major difference between the B2 NiAl and Reynaud's structure Ni₂Al is the replacement of a plane of Al atoms with Ni atoms (figure 1(b)). This suggests that a major factor for the instability of this Ni₂Al structure originates from this replacement. Since Ni–Ni and Ni–Al bonds are very similar to each other, one does not expect that the replacement of Al by Ni atoms in B2 structure should make any major contribution to the instability of the system, when only considering first-nearest-neighbour interactions. As one can see from figure 8, the interactions up to first-nearest-neighbour shells tend to stabilize Reynaud's structure. However, in Reynaud's structure Al atoms have two different types of second-nearest neighbour. Half (three atoms) of the second-nearest neighbours are Ni atoms and the other half are Al atoms. Since the Ni–Al bonds are stronger than Al–Al bonds, there are unbalanced interactions which force the Al atoms to move towards the Ni atoms (figure 1(c)). In the rearranged system, some of the Ni atoms and Al atoms are changed (cf. figure 3(b)), and a weak Al–Al bond (as a

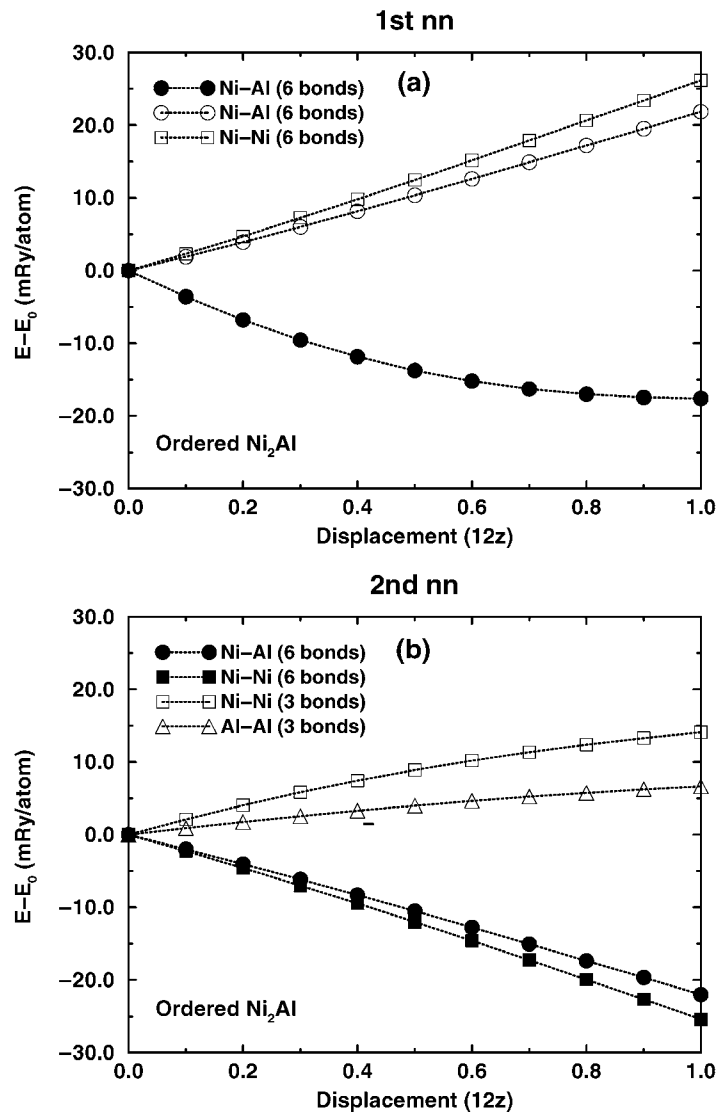


Figure 8. Pair potential of each bond for ordered Ni_2Al system. (a) First-nearest neighbours and (b) second-nearest neighbours. Filled and unfilled signs refer to the approaching and non-approaching atoms, respectively. The legend specifies the type of bond (e.g., Ni-Al) and the following number in parentheses gives the number of these types of bond in the unit cell. We give the additional bond-number information since the number of bonds times the energy of the bond gives the total energy contribution of that bond. Note that there are two inequivalent types of first-nearest-neighbour Ni-Al bond that give different energies because they have different bond lengths.

second-nearest neighbour) is replaced by a strong Ni-Al bond. Shuffling the atoms in an ω -type transformation now increases the distance between a pair of second-nearest-neighbour Ni and Al atoms, which consequently increases the energy of the system, and thus makes the bcc structure more stable.

A careful comparison of the placement of Al-Al bonds in pure B2 and ordered Ni_2Al (cf. figure 1) shows that this same argument works for explaining the stability of bcc NiAl with

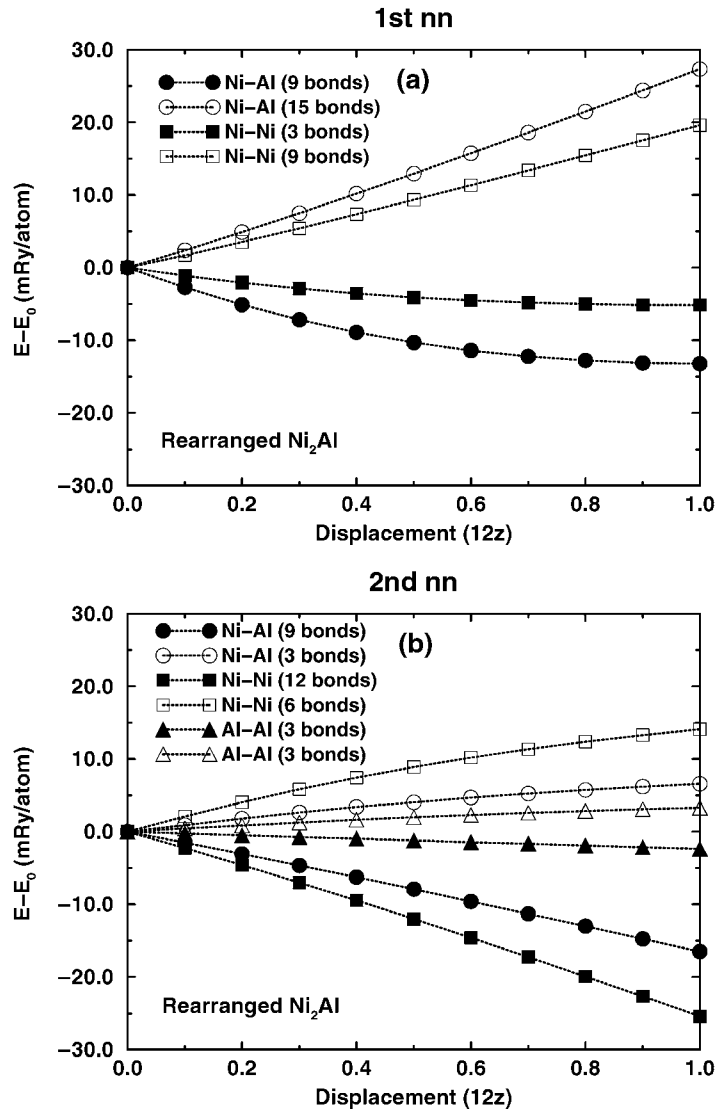


Figure 9. Pair potential of each bond for rearranged Ni₂Al system. (a) First-nearest neighbours and (b) second-nearest neighbours. Filled and unfilled signs refer to the approaching and non-approaching atoms, respectively. Refer to figure 8 for additional information about the notation used in this figure.

respect to an ω -phase transformation. In the B2 (CsCl) structure, every other plane is an Al plane of atoms. Hence, the weak Al–Al second-nearest-neighbour bonds are balanced above and below. Without an asymmetry, there is no driving force for the ω -type collapse of planes, and the bcc structure remains the most stable.

In general, a pair-potential description of the martensitic phase transformation has turned out to be rather disappointing. While it is adequate to suggest the role of the unbalanced forces on the Al atoms, it appears to be highly structure dependent and not as quantitative as we would like (e.g., the fits for NiAl are not nearly as good as for Ni₂Al). Also, the relatively small

energies involved in the phase transformation involve a delicate balance of many different atomic forces, which limit the qualitative types of conclusion one can draw from such an analysis. For these reasons we would not recommend this type of study for other related systems.

5. Conclusions

We have performed first-principles calculations and a pair-potential model to understand the bonding and phase stability of bcc structures with respect to an ω -phase transformation. Our *ab initio* calculations showed that NiAl is stable in the bcc phase, and that the Ni₂Al phase has an incomplete ω -type structure as its ground state. The calculated value for the amount of the shuffle is within the range of experimental estimations. The first-principles calculations also show that rearranging the atoms within a supercell tends to inhibit ω -phase type transformations for Ni₂Al, which supports the suggestion of a combined displacive/ordering transformation mechanism [2, 3] for the formation of this phase. A pair-potential model would interpret this inhibiting tendency in terms of weak second-nearest-neighbour Al–Al bonds relative to much stronger Ni–Ni and Ni–Al bonds.

Acknowledgments

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