Embedded-atom potential for Ni-Al alloy

Gang Wang a and Yishuang Xu b
TianJin college, University of Science and Technology Beijing, Tianjin 301830, China.

a wangsoft007@126.com, b xyshuang_w@126.com

Abstract. We construct a new embedded-atom potential for Ni-Al system. The lattice constants, cohesive energies, elastic constants, vacancy formation energies, stacking fault energies and equations of state of Ni and Al are included in the fitting process of potentials for pure Ni and pure Al. The cross-interaction potential is fitted to the lattice constants, cohesive energies, elastic constants of Ni3Al and NiAl and the energies of (100) APB and (111) SISF of Ni3Al. The potential accurately reproduces the various physical properties of Ni, Al, Ni3Al and NiAl phases. The results of the new embedded-atom potential and other embedded-atom potentials are compared and discussed in detail.

Keywords: EAM potential, Structural stability, Point defects, Planar defects.

1. Introduction

Ni-Al intermetallic compounds mainly include five phases: Ni3Al, Ni5Al3, NiAl, Ni2Al3 and NiAl3. Among them, L12-type Ni3Al and B2-type NiAl are considered as high temperature structural materials because of their high melting point and low density [1-2]. Therefore, in recent years, people have extensively studied their physical properties in theory. The dislocation, creep and fracture behavior of the alloy can be better understood by atomistic simulation, and the reliability of atomic-level simulation depends on the interatomic potential. The most widely used potential in the atomistic simulation of intermetallic compounds is the many-body potential based on the embedded atom method (EAM).

Several EAM potentials for Ni-Al system have been proposed. The most famous of them are presented by Voter and Chen [3], and Mishin [4, 5]. Among them, Voter-Chen (VC) EAM and Mishin-2004 (M04) EAM [5] are proposed for Ni3Al. The calculated lattice constants, cohesive energies, elastic constants, point defect properties and antiphase boundary (APB) energies of Ni3Al by these three EAM potentials agree with the experimental data. However, the calculated NiAl properties are often different from the experimental data, such as: the elastic constants of NiAl calculated by VC EAM and M04 EAM are about 50% larger than the experimental values, and the calculated point defect properties of NiAl deviate from the experimental results. Moreover, the (111) complex stacking fault (CSF) energies calculated by VC EAM and M04 EAM are less than the corresponding (111) APB energy, which is inconsistent with the experimental results. The Mishin-2002 (M02) EAM [4] is proposed for NiAl, the calculated properties of NiAl agree well with the experimental results. However, the maximum error between the calculated elastic constants of Ni3Al and the experimental data is about 50%, and the
calculated (111) APB energy of Ni₃Al, 298 mJ/m², is much larger than the experimental value, 175 mJ/m² [6].

In this paper, we first obtained a new EAM potentials of Ni-Al system by fitting the physical properties of Ni, Al, Ni₃Al and NiAl. Then, the various properties of Ni, Al, Ni₃Al and NiAl are calculated, and the results are discussed.

2. Development of EAM potential

The EAM model in this work within the framework of the original EAM theory [7]. The total energy of crystal can be written as

\[
E_{\text{tot}} = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{i,j(i\neq j)} \phi_{ij}(r_{ij})
\]

\[
\rho_i = \sum_j f_j(r_{ij})
\]

Where \( F_i \) is the embedding energy of atom \( i \), \( \rho_i \) is the host electron density at atom \( i \), \( \phi_{ij} \) is the pair potential between atoms \( i \) and \( j \), \( r_{ij} \) is the distance between atoms \( i \) and \( j \), \( f_j \) is the atomic electron density contributed by atom \( j \). For a binary system A-B, seven potential functions, namely \( F_A(\rho) \), \( F_B(\rho) \), \( f_A(r) \), \( f_B(r) \), \( \phi_{AA}(r) \), \( \phi_{BB}(r) \) and \( \phi_{AB}(r) \), must be determined. All these functions can be obtained by fitting to properties of element A, element B and A-B alloys.

The embedding energy \( F_A(\rho) \) and \( F_B(\rho) \) are based on the universal equation proposed by Banerjea and Smith [8]:

\[
F(\rho) = -F_0 [1 - \ln(\frac{\rho}{\rho_e})^n] \left( \frac{\rho}{\rho_e} \right)^n
\]

Where \( F_0 = E_c - E_v \), \( E_c \) is the cohesive energy of pure element, \( E_v \) is the unrelaxed vacancy formation energy of pure element, \( \rho_e \) is the equilibrium value of host electron density \( \rho \), \( n \) is an adjustable parameter.

The pair potential functions \( \phi_{AA}(r) \), \( \phi_{BB}(r) \) and \( \phi_{AB}(r) \) are taken as a polynomial function

\[
\phi(r) = (k_1 r^{-12} + k_2 r^{-6} + k_3 r^{-3} + k_4 r^{-2} + k_5 r^{-1} + k_6 + k_7 r + k_8 r^6) \Psi \left( \frac{r - r_c}{h_1} \right)
\]

Where \( \Psi(x) \) is a cutoff function defined as

\[
\Psi(x) = \begin{cases} x^4, & x < 0, \\ \frac{1}{1 + x^4}, & x \geq 0. \end{cases}
\]

\( k_i (i = 1, 2, \ldots, 8), \) \( r_c \) and \( h_1 \) are parameters for fitting.

The atomic electron density functions \( f_A(r) \) and \( f_B(r) \) are parameterized in an exponential form.
\[ f(r) = \exp(p_1 + p_2r + p_3r^2 + p_4r^3 + p_5r^4 + p_6r^5)\psi\left(\frac{r - r_c}{h_2}\right) \]  

(6)

Where \( p_i (i = 1, 2, \ldots, 6) \), \( r_c \) and \( h_2 \) are adjustable parameters.

### Table 1. Parameters of the EAM potentials for Ni, Al and Ni-Al.

| Parameter         | Ni                      | Al                      | Ni-Al                   |
|-------------------|-------------------------|-------------------------|-------------------------|
| \( k_1 (\text{eV}\cdot\text{Å}^{12}) \) | -1.01641                | -5.0039×10³             | 6.56051×10³             |
| \( k_2 (\text{eV}\cdot\text{Å}^6) \) | 9.13085×10²             | 9.89489×10²             | -3.39649×10³            |
| \( k_3 (\text{eV}\cdot\text{Å}^3) \) | -5.77191×10²             | -6.07473×10²             | 4.98030×10³             |
| \( k_4 (\text{eV}\cdot\text{Å}^2) \) | 4.57336×10²             | 4.53629×10²             | -5.09894×10³            |
| \( k_5 (\text{eV}\cdot\text{Å}) \) | -1.46211×10²             | -1.35644×10²             | 2.07449×10³             |
| \( k_6 (\text{eV}) \) | 2.17674×10¹             | 1.89981×10¹             | -3.90795×10²            |
| \( k_7 (\text{eV}\cdot\text{Å}^{-1}) \) | -1.26219                | -1.05203                | 2.86639×10¹             |
| \( k_8 (\text{eV}\cdot\text{Å}^{-6}) \) | 2.54717×10⁻⁶             | 2.37244×10⁻⁶             | -2.09872×10⁻⁴            |
| \( h_1 (\text{Å}) \) | 1.77063×10⁻¹             | 1.60313×10⁻¹             | 1.99167                 |
| \( r_c (\text{Å}) \) | 6.86116                 | 5.97079                 | 6.07056                 |
| \( p_1 (\text{Å}^{-1}) \) | 2.43265×10¹             | 1.11001×10²             | 1.1001×10²              |
| \( p_2 (\text{Å}^{-1}) \) | -4.80849×10¹             | -1.95576×10²             | -1.95576×10²            |
| \( p_3 (\text{Å}^{-2}) \) | 3.11215×10¹             | 1.28529×10²             | 1.28529×10²             |
| \( p_4 (\text{Å}^{-2}) \) | -9.72395                | -4.10793×10¹             | -4.10793×10¹            |
| \( p_5 (\text{Å}^{-4}) \) | 1.42614                 | 6.30792                 |                          |
| \( p_6 (\text{Å}^{-8}) \) | -7.91941×10⁻²            | -3.74326×10⁻¹            |                          |
| \( h_2 (\text{Å}) \) | 2                       | 0.15                    |                          |
| \( F_0 (\text{eV}) \) | 2.725                   | 2.89                    |                          |
| \( n \) | 0.6                     | 0.39                    |                          |

Potential functions of pure elements Ni and Al, namely \( F_{Ni}(\rho) \), \( F_{Al}(\rho) \), \( f_{Ni}(r) \), \( f_{Al}(r) \), \( \phi_{Ni}(r) \) and \( \phi_{Al}(r) \), can be determined by fitting the vacancy formation energy, cohesive energy, lattice constant, elastic constants, energy difference between fcc and hcp structure and equations of state. The cross-interaction function \( \phi_{AlNi}(r) \) can be obtained by fitting the cohesive energies, lattice constants and elastic constants of Ni₃Al and NiAl. Because the planar defects have an important influence on the mechanical properties of the alloy, we should consider the planar defects in the fitting. The (100) APB energy of Ni₃Al is related to the energy difference of the L1₂ structure and the D0₂₂ structure [9], the (111) SISF energy of Ni₃Al is related to the energy difference of the L1₂ structure and the D0₁₉ structure [5]. We also include the energy differences mentioned above when fitting the potential parameters.

The fitting results of potential parameters are listed in Table 1. In this work, all the calculations using the EAM potentials for the properties of elements and alloys are carried out by LAMMPS[10].

### 3. Properties of Ni and Al

The lattice constants \( (a_0) \), cohesive energies \( (E_c) \), elastic constants \( (C_{ij}) \), vacancy formation energies \( (E'_v) \), vacancy migration energies \( (E''_v) \), stacking fault energies \( (E'_{sf}) \), twin boundary energies \( (E'_{tb}) \) and surface energies \( (SE) \) of Ni and Al are calculated by the present EAM. And the results are compared with the experimental data and the results of VC EAM and M04 EAM in Table 2. It is clearly that the results of the three EAM potentials agree well with the experimental data. Moreover, the elastic constants
obtained by the present EAM agree better with the experimental data than those of VC EAM and M04 EAM. Therefore, the present EAM potential can effectively describe the properties of Ni and Al.

### Table 2. Properties of Ni and Al.

|       | Ni | Al |
|-------|----|----|
|       | Exp. | present | VC | M04 | Exp. | present | VC | M04 |
| \(a_0\) (Å) | 3.524<sup>a</sup> | 3.524 | 3.520 | 3.520 | 4.05<sup>a</sup> | 4.05 | 4.05 | 4.05 |
| \(E_c\) (eV) | 4.44<sup>a</sup> | 4.44 | 4.45 | 4.45 | 3.39<sup>a</sup> | 3.39 | 3.36 | 3.36 |
| \(C_{11}\) (GPa) | 261.2<sup>a</sup> | 260.9 | 244 | 241.3 | 114.3<sup>a</sup> | 114.5 | 107 | 116.8 |
| \(C_{12}\) (GPa) | 150.8<sup>a</sup> | 150.4 | 149 | 150.8 | 61.9<sup>a</sup> | 61.9 | 65.2 | 60.1 |
| \(C_{44}\) (GPa) | 131.7<sup>a</sup> | 131.6 | 126 | 127.3 | 31.6<sup>a</sup> | 31.4 | 32.2 | 31.7 |
| \(E_{\text{sf}}\) | 1.55<sup>b</sup> | 1.56 | 1.56 | 1.57 | 0.67<sup>b</sup> | 0.67 | 0.63 | 0.71 |
| \(E_{\text{tb}}\) | 1.12<sup>d</sup> | 1.12 | 0.98 | 1.19 | 0.65<sup>b</sup> | 0.41 | 0.3 | 0.65 |
| \(E_{\text{se}}\) | 125<sup>e</sup> | 107 | 58 | 134 | 166<sup>e</sup> | 99 | 76 | 115 |
| \(E_{\text{se}}\) | 43<sup>e</sup> | 53 | 30 | 68 | 75<sup>e</sup> | 49 | 42 | 63 |
| \(SE_{110}\) | 2240<sup>e</sup> | 1677 | 1977 | 2087 | 980<sup>e</sup> | 761 | 707 | 672 |
| \(SE_{100}\) | 2240<sup>e</sup> | 1545 | 1754 | 1936 | 980<sup>e</sup> | 959 | 855 | 823 |
| \(SE_{111}\) | 2240<sup>e</sup> | 1425 | 1621 | 1759 | 980<sup>e</sup> | 792 | 607 | 601 |

<sup>a</sup> Ref. [11].<sup>b</sup> Ref. [12].<sup>c</sup> Ref. [13].

4. Properties of Ni3Al and NiAl

4.1. Lattice constant, cohesive energy and elastic constants.

The calculated values of the lattice constant, cohesive energy and elastic constants of Ni3Al and NiAl are listed in Table 3. For comparison, the results for the VC EAM, M02 EAM and M04 EAM and the experimental data are also shown in Table 3. It can be seen from Table 3 that the results of the present EAM agree well with the experimental data. The elastic constants of Ni3Al are not included in the fitting of the M02 EAM, and the elastic constants of NiAl are not included in the fitting of the VC EAM and the M04 EAM, so the corresponding calculated values have a large difference from the experimental data.

### Table 3. Lattice constants, cohesive energies and elastic constants of Ni3Al and NiAl.

|       | Ni3Al | NiAl |
|-------|-------|------|
|       | Exp. | present | VC | M02 | M04 | Exp. | present | VC | M02 | M04 |
| \(a_0\) (Å) | 3.567<sup>a</sup> | 3.563 | 3.573 | 3.526 | 3.571 | 2.88<sup>d</sup> | 2.88 | 2.87 | 2.86 | 2.86 |
| \(E_c\) (eV) | 4.57<sup>b</sup> | 4.61 | 4.59 | 4.60 | 4.63 | 4.50<sup>b</sup> | 4.46 | 4.38 | 4.47 | 4.5 |
| \(C_{11}\) (GPa) | 230<sup>c</sup> | 233 | 246 | 284 | 236 | 199<sup>e</sup> | 197 | 278 | 200 | 297 |
| \(C_{12}\) (GPa) | 150<sup>c</sup> | 148 | 137 | 229 | 154 | 137<sup>e</sup> | 139 | 184 | 140 | 206 |
| \(C_{44}\) (GPa) | 131<sup>c</sup> | 129 | 123 | 105 | 127 | 116<sup>e</sup> | 116 | 178 | 120 | 171 |

<sup>a</sup> Ref. [14].<sup>b</sup> Ref. [15].<sup>c</sup> Ref. [3].<sup>d</sup> Ref. [11].<sup>e</sup> Ref. [16].

4.2. Structural stability.

The lattice constants and cohesive energies of several alternative structures of L12-Ni3Al and B2-NiAl are calculated by the present EAM. The lattice constants of the alternative structure and the energy differences between the alternative structure and the original structure are shown in Table 4. For comparison, the results of the first principles are also listed in the table. All of the first principles calculations in this work are based on the CASTEP software package [17], and the GGA-PBE exchange correlation functional is adopted [18]. It can be seen from Table 6 that the calculated results for the present EAM are in good agreement with the first principles calculations. The lattice constants are
basically the same, and the ordering of cohesive energy in different structures is the same. The L1_2 structure is the lowest-energy structure of Ni_3Al, and the B2 structure is the lowest-energy structure of NiAl. It is shown that the structural stability predicted by the present EAM is accurate and correct.

### Table 4. Lattice constants of the alternative structures of L1_2-Ni_3Al and B2-NiAl, and energy differences (ΔEc) between the alternative structures and the original structure. If two lattice constant values are given, separated by commas, they denote a and c, respectively.

| Phase  | Structure | Present EAM | CASTEP* |
|--------|-----------|-------------|---------|
|        |           | a_0 (Å)    | ΔEc (eV) | a_0 (Å)    | ΔEc (eV) |
| Ni_3Al | D0_19     | 5.047, 4.102 | 0.001    | 5.104, 4.103 | 0.012    |
|        | D0_23     | 3.553, 14.270 | 0.013    | 3.635, 14.054 | 0.015    |
|        | D0_52     | 3.543, 7.149  | 0.027    | 3.677, 6.902  | 0.033    |
|        | D0_6      | 5.959        | 0.698    | 5.713        | 0.061    |
| NiAl   | B20       | 5.814        | 0.065    | 4.647        | 0.014    |
|        | L1_0^b    | 2.567, 3.630  | 0.074    | 2.590, 3.663  | 0.132    |
|        | L1_1      | 2.677, 11.833 | 0.169   | 2.745, 11.759 | 0.228    |
|        | B32       | 5.737        | 0.181    | 5.877        | 0.312    |
|        | B1        | 4.754        | 0.521    | 4.885        | 0.623    |

*Calculated in this work. ^b After relaxation, the L1_0 structure changes into the B2 structure. So we have a static calculation with the same volume as the B2 structure and c/a=√2.

#### 4.3. Point defects.

The perfect crystal structure can only exist at the condition of absolute zero and stoichiometric composition. Therefore, there are many kinds of defects in the alloy, among which point defects are very common. The presence of point defects has an important influence on the physical and mechanical properties of intermetallic compounds. Neglecting interstitial atoms, Ni_3Al and NiAl support four types of point defect: vacancies in the Ni sublattice (V_Ni), vacancies in the Al sublattice (V_Al), Al antisites in the Ni sublattice (Al_Ni), Ni antisites in the Al sublattice (Ni_Al). The point defect formation energies of Ni_3Al and NiAl are calculated by the following equation:

\[
E_f(V_{Ni}) = E_{rel} - E_{per} + E(Ni) \tag{7}
\]

\[
E_f(V_{Al}) = E_{rel} - E_{per} + E(Al) \tag{8}
\]

\[
E_f(Al_{Ni}) = E_{rel} - E_{per} + E(Ni) - E(Al) \tag{9}
\]

\[
E_f(Ni_{Al}) = E_{rel} - E_{per} + E(Al) - E(Ni) \tag{10}
\]

Where \(E_{rel}\) is the energy of the system with point defect, \(E_{per}\) is the energy of the system with perfect lattice, \(E(Al)\) and \(E(Ni)\) are the energies of Al atom and Ni atom in perfect lattice respectively. The results are compared with the results of M02 EAM and M04 EAM in Table 5. If the formation energy of antisite defect is lower than that of the vacancy defect, it means that defects are mainly antisite defects; Otherwise, it means that defects are mainly vacancy defects. The experimental results show that: for Ni_3Al, defects are mainly Ni antisite defects on the Ni-rich side and Al antisite defects on the Al-rich side; for NiAl, defects are mainly Ni antisite defects on the Ni-rich side and Ni vacancy defects on the Al-rich side [19]. The results of the three EAM potential are the same as the experimental results.
Table 5. Point defect formation energies of Ni$_3$Al and NiAl.

|                  | Ni$_3$Al | NiAl |
|------------------|----------|------|
|                  | present  | M02  | M04  | present | M02  | M04  |
| $V_{Ni}$ (eV)    | 1.72     | 1.63 | 1.63 | 1.63    | 1.47 |
| $V_{Al}$(eV)     | 1.71     | 1.81 | 1.05 | 2.08    | 1.14 |
| $Al_{Ni}$ (eV)   | 0.81     | 0.88 | 1.94 | 1.11    | 2.04 |
| $Ni_{Al}$ (eV)   | 0.23     | 0.79 | -0.65| 1.65    | 0.13 |

4.4. Planar defects.
The planar defects in alloys have an important influence on their mechanical properties. There are three main types of planar defects: APB, CSF and SISF. The energies of (111) APB, CSF, SISF and (110) APB for Ni$_3$Al, and the energies of (110) APB and (211) APB for NiAl are calculated by the present EAM. The calculation results are shown in Table 6. For comparison, the experimental values and the results of M04 EAM are also listed in the Table 6. As can be seen from Table 6, the calculated results of the present EAM are in good agreement with the experimental results. For the VC EAM and M04 EAM, the calculated (111) APB energy is greater than the (111) CSF energy, this is contrary to the experimental results. And the result of M02 EAM is quite different from that of the experiment. These indicate that the present EAM potential can better describe the planar defects of Ni$_3$Al and NiAl.

Table 6. Energies (in mJ/m$^2$) of planar defects of Ni$_3$Al and NiAl.

| Fault       | Exp. | Present | VC  | M02 | M04 |
|-------------|------|---------|-----|-----|-----|
| Ni$_3$Al    |      |         |     |     |     |
| (111) APB   | 175$^a$ | 188     | 142 | 298 | 252 |
| (111) CSF   | 235$^a$ | 232     | 120 | 324 | 202 |
| (111) SISF  | 6$^a$  | 5       | 13  | 60  | 51  |
| (100) APB   | 104$^a$ | 134     | 83  | 55  | 80  |
| NiAl        |      |         |     |     |     |
| (110) APB   | 500$^b$ | 404     | 530 | 530 | 591 |
| (211) APB   | 750$^b$ | 440     | 620 | 700 | 690 |

$^a$[7]. $^b$[20].

5. Summary
In the construction of the present EAM, the properties used for fitting include the lattice constants, cohesive energies, elastic constants, vacancy formation energies, stacking fault energies and equation of state of pure elements Ni and Al, the lattice constants, cohesive energies, elastic constants of Ni$_3$Al and NiAl and the energies of (100) APB and (111) SISF of Ni$_3$Al.

The lattice constants, cohesive energies, elastic constants, structural stability, point defects and planar defects of Ni, Al, Ni$_3$Al and NiAl calculated by the present EAM agree well with the experimental results or the first-principles results. Compared with the VC EAM, M02 EAM and M04 EAM, the present EAM has improved the calculation results of the planar defects energies of Ni$_3$Al and the elastic constants of NiAl. All these indicate that the present EAM potential can describe the properties of Ni-Al system more effectively.

References
[1] L.Y. Sheng, W. Zhang, J.T. Guo, et al. Microstructure and mechanical properties of Ni$_3$Al fabricated by thermal explosion and hot extrusion. Intermetallics. Vol. 17 (2009) No. 7, p. 572-577.
[2] Ram Darolia. NiAl alloys for high-temperature structural applications. JoM. Vol. 43 (1991) No. 3, p. 44-49.
[3] A.F. Voter, S.P. Chen. Accurate Interatomic Potentials for Ni, Al and Ni$_3$Al. MRS Online Proceedings Library Archive. Vol. 82 (1986).
[4] Y. Mishin, M.J. Mehl, D.A. Papaconstantopoulos. Embedded-atom potential for B2-NiAl.
7

Physical Review B. Vol. 65 (2002) No. 22, p. 224114.

[5] Y. Mishin. Atomistic modeling of the γ and γ'-phases of the Ni–Al system. Acta Materialia. Vol. 52 (2004) No. 6, p. 1451-1467.

[6] H.P. Karnthaler, E.T. Mühlbacher. The influence of the fault energies on the anomalous mechanical behaviour of Ni3Al alloys. Acta Materialia. Vol. 44 (1996) No. 2, p. 547-560.

[7] M.S. Daw, M.I. Baskes. Semiempirical, Quantum Mechanical Calculation of Hydrogen Embrittlement in Metals. Physical Review Letters. Vol. 50 (1983) No. 17, p. 1285-1288.

[8] A. Banerjea, J.R. Smith. Origins of the universal binding-energy relation. Physical review B. Vol. 37 (1988) No. 12, p. 6632.

[9] A.T. Paxton, Y.Q. Sun. The role of planar fault energy in the yield anomaly in L12 intermetallics. Philosophical Magazine A. Vol. 78 (1998) No. 1, p. 85-104.

[10] S. Plimpton. Fast Parallel Algorithms for Short-Range Molecular Dynamics. Journal of Computational Physics. Vol. 117 (1995) No. 1, p. 1-19.

[11] C. Kittel. Introduction to Solid State Physics. John Wiley & Sons, 1976, p.15-64.

[12] W. Schäule, R. Scholz. Proceedings of Yamada conference on point defects and defect interactions in metals. University of Tokyo Press, 1982, p. 257-259.

[13] L.E. Murr. Interfacial phenomena in metals and alloys. Addison-Wesley Pub, 1975, p. 376.

[14] F.A. Maurer. Compression studies of a nickel-based superalloy, MAR-M200, and of Ni3Al. Journal of Applied Physics. Vol. 58 (1985) No. 10, p. 3727-3730.

[15] R. Hultgren. Selected Values of the Thermodynamic Properties of Binary Alloys. National Standard Reference Data System, 1973.

[16] N. Rusović, H. Warlimont. The elastic behaviour of β2-NiAl alloys. Physica Status Solidi (a). Vol. 44 (1977) No. 2, p. 609-619.

[17] M.D. Segall. First-principles simulation: ideas, illustrations and the CASTEP code. Journal of Physics: Condensed Matter. Vol. 14 (2002) No. 11, p. 2717.

[18] J.A. Chevary. Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. Physical Review B. Vol. 46 (1992) No. 11, p. 6671-6687.

[19] A. Taylor, N.J. Doyle. Further studies on the nickel–aluminium system. I. β-NiAl and δ-Ni2Al3 phase fields. Journal of Applied Crystallography. Vol. 5 (1972) No. 3, p. 201-209.

[20] P. Veyssière, R. Noebe. Weak-beam study of <111> superlattice dislocations in NiAl. Philosophical Magazine A. Vol. 65(1992) No. 1, p. 1-13.