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STUDY OF INTERACTION POTENTIAL AND FORCE CONSTANTS OF FCC CRYSTALS CONTAINING N IMPURITY ATOMS

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Abstract. A new procedure for description and calculation of the interaction potential and force constants for fcc crystals containing an arbitrary number n of impurity atoms have been developed. Analytical expressions for the effective atomic interaction potential, the single-bond and effective spring constants have been derived. They depend on the number of the impurity atoms and approach those derived by using anharmonic correlated Einstein model, if all the impurity atoms are taken out or they replace all the host atoms. Numerical results for Ni doped by Cu atoms show significant changes of the interaction potential and spring constants of the substance if the number of impurity atoms is changed.

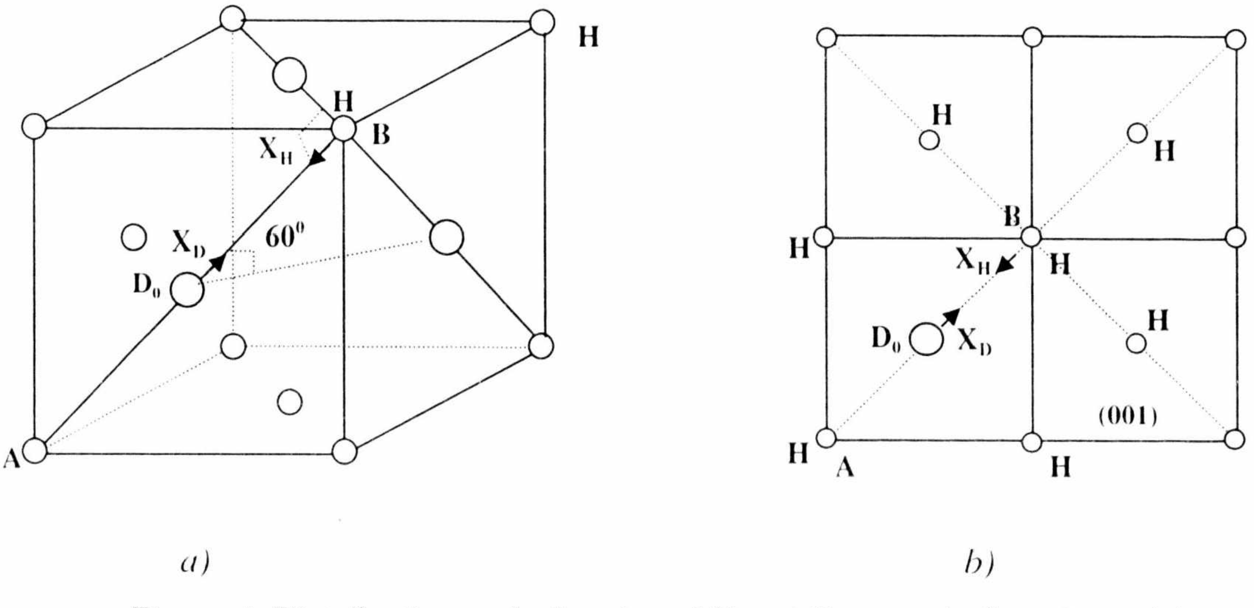
1. Introduction

Interaction potential and force constants are very important for studying a lot of physical properties such as thermodynamic parameters of the crystals. They are contained in the first cummulant or net thermal expansion, the second cumulant or Debye-Waller factor, the third cumulant, and the thermal expansion expansion coefficient, which are investigated intensively in the X-ray absorption fine structure (XAFS) experiment and theory [1-11]. It is also very important to sudy thermodynamic properties of materials containing impurity atoms and of alloy systems [12, 17-19]. Some investigations for crystals containing one impurity atom have been done [17-19]. But more than one impurity atom can be doped into a crystal. This case can lead to the development of procedures for studying thermodynamic properties of alloys with nano structure which are often semiconductors containing some components with different atomic sortes.

The purpose of this work is to develop a new procedure for description and calculation of the interaction potential and force constants of fcc crystals containing some impurity atoms, where one impurity atom [17-19] is only an special case of this theory. Our development is derivation of the analytical expressions for the effective atomic interaction potential, the single-bond and the effective spring constants for the case when the cluster involves one or more impurity atons. Using the atomic distribution of the host (H) atoms and the dopant (D) atoms in a cluster one can deduce the percentage of these constituent elements in the substance or in an alloy. All these expressions are different if the number of impurity atoms changes so that one can deduce the results for the case with different percentages of component elements of which an alloy consists. The results in the case if all impurity atoms are taken out or in the case if all host atoms are replaced by the impurity atoms are reduced to those derived by using the anharmonic correlated Einstein model [7] for the pure materials. Numerical calculations have been carried out for Ni crystal doped by one or more Al impurity atoms, and the results are compared to those of the pure materials.

2. Formalism

We consider a fcc crystal doped by some impurity atoms or dopants (D), the D atoms replace the host (H) atoms located in the centre of crystal planes. Supposed that the XAFS process is taken place in the surface (001) between the D atom (indicated by D_0) in the centre and the H atom located at the position B (indicated by H_B) as described in Figure 1a.



a) *b)*

Figure 1. Distribution and vibration of H and D atoms in fcc volume (a) and in its (001) surface (b).

Now move the D_0 atom by an amount X_D along the line AB, then the H_B atom moves backward by an amount X_H so that the mass centre remains unchanged, the other atoms are fixed. We have relations

$$X_D M_D = X_H M_H \quad \Rightarrow \quad \mathrm{X_H} = \frac{M_D}{M_H} X_D = \varepsilon . X_D \,, \; \varepsilon = \frac{M_D}{M_H} \,, \tag{1}$$

where M_H, M_D are the mass of H and D atom, respectively.

This motion leads to increasing the potential energy. The contributions of the springs in the surface (001) are caused mainly by the atoms in the bond AB, and those of the springs penperdicular to AB are negligible (see Figure 1b). Therefore, they consist of contributions of the spring $D\text{-}H_A$ by the value $K_{HD}X_D^2/2$; of the spring $D\text{-}H_B$ by $K_{HD}(X_H+X_D)^2/2$; and of the spring between H_B and H on the extended AB by $K_{HH}X_H^2/2$.

Hence, the contribution of the atoms on the plane is given by

$$V_P = \frac{1}{2}K_{HD}X_D^2 + \frac{1}{2}K_{HD}(X_H+X_D)^2 + \frac{1}{2}K_{HH}X_H^2. \tag{2}$$

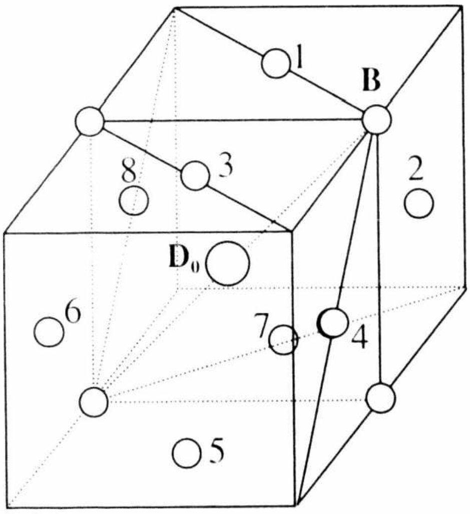


Figure 2. The neighbors of D_0 atom.

Besides bonding with 4 H atoms at 4 verteses of the plane (001), the D_0 atom is bonded with 8 other neighboring atoms (see Figure 2) located in the centre of 8 neighboring planes counting from 1 to 8. They are numbered by 1, 2, 3, 4 and are the neighbors of the H_B atom. The remaining atoms are the neighbors of D_0, but they are also the neighbors of the H_B atom. Supposed that n is the total number of dopant atoms in the two neighboring lattices of D_0 atom and among the atoms at positions 1, 2, 3, 4 there are n_1 dopant (D) atoms, then among the positions 5, 6, 7, 8 there are $n_2 = n - 1 - n_1$ dopant (D) atoms ($0 \le n_1, n_2 \le 4$).

The bond linking the D_0 atom with each of the atoms fom 1 to 4 builds with X_D an angle of 60^0. that is why the effective displacement of the bond from D_0 to these atoms is given by $X_D\cos(60^0) = X_D/2$. The bond from D_0 to the atoms numbered by 5, 6, 7, 8 builds with X_D an angle of 120^0, that is why the effective displacement of the bond from D_0 to these atoms is given by $X_D\cos(120^0) = -X_D/2$. Hence, the potential contributed by these 8 atoms is equal to

$$\begin{aligned} V_{DO} &= (n_1+n_2).\frac{1}{2}K_{DD}(\frac{1}{2}X_D)^2 + (8-n_1-n_2).\frac{1}{2}K_{HD}(\frac{1}{2}X_D)^2 \\ &= \frac{n_1+n_2}{8}K_{DD}X_D^2 + \frac{(8-n_1-n_2)}{8}K_{HD}X_D^2 \end{aligned} \tag{3}$$

The line bonding H_B with 4 atoms numbered by 1, 2, 3, 4 also builds with X_H an angle of 60^0 and the line bonding H_B with 4 other out of the surface (001) neighbors of H_B builds with X_H an angle of 120^0, then the potential contributed by these interactions is given by

$$V_{HO} = \frac{n_1}{8} K_{HD} X_H{}^2 + \frac{(4-n_1)}{8} K_{HH} X_H{}^2 + 4 \cdot \frac{1}{8} \cdot K_{HH} X_H{}^2$$

$$= \frac{n_1}{8} K_{HD} X_H{}^2 + \frac{(8-n_1)}{8} K_{HH} X_H{}^2 . \tag{4}$$

Therefore, the total potential increase is the sum of all the above contributions

$$\begin{aligned} V_{tot} &= V_P + V_{DO} + V_{HO} \\ &= \frac{1}{2} K_{HD} X_D{}^2 + \frac{1}{2} K_{HD} (X_H + X_D)^2 + \frac{1}{2} K_{HH} X_H{}^2 \\ &+ \frac{n_1 + n_2}{8} K_{DD} X_D{}^2 + \frac{(8 - n_1 - n_2)}{8} K_{HD} X_D{}^2 \\ &+ \frac{n_1}{8} K_{HD} X_H{}^2 + \frac{(8-n_1)}{8} K_{HH} X_H{}^2 \end{aligned} \tag{5}$$

Substituting (1) into (5) we obtain

$$\begin{aligned} V_{tot} &= \frac{1}{2} K_{HD} X_D{}^2 + \frac{1}{2} K_{HD} (\varepsilon + 1)^2 X_D{}^2 + \frac{1}{2} \varepsilon^2 K_{HH} X_D{}^2 \\ &+ \frac{n_1 + n_2}{8} K_{DD} X_D{}^2 + \frac{(8 - n_1 - n_2)}{8} K_{HD} X_D{}^2 \\ &+ \frac{n_1 \varepsilon^2}{8} K_{HD} X_D{}^2 + \frac{(8-n_1)\varepsilon^2}{8} K_{HH} X_D{}^2 \end{aligned}$$

or

$$V_{tot} = \frac{1}{8} \left\{ \begin{aligned} &(12 - n_1)\varepsilon^2 K_{HH} + (n_1 + n_2) K_{DD} + \\ &+ [4(\varepsilon+1)^2 + n_1 \varepsilon^2 + 12 - n_1 - n_2] K_{HD} \end{aligned} \right\} X_D^2 . \tag{6}$$

Using $X = X_H + X_D = (\epsilon + 1).X_D$ and comparing (6) to $V_{tot} = \frac{1}{2} K_{\text{eff}} X^2$ the effective force constant is resulted as

$$\begin{aligned} K_{\text{eff}} &= \frac{1}{4(\varepsilon+1)^2} \left\{ (12 - n_1)\varepsilon^2 K_{HH} + (n_1 + n_2) K_{DD} + [4(\varepsilon+1)^2 + n_1 \varepsilon^2 + 12 - n_1 - n_2] K_{HD} \right\} \\ &= \frac{1}{4(\varepsilon+1)^2} \left\{ (12 - n_1)\varepsilon^2 K_{HH} + (n-1) K_{DD} + [4(\varepsilon+1)^2 + n_1 \varepsilon^2 + 13 - n] K_{HD} \right\} \end{aligned} \tag{7}$$

For the case without impurity, i. e., $\epsilon = 1$, $K_{DD} = K_{HD} = K_{HH}$, we obtain

$$K_{\text{eff-pure}} = 2.5 K_{HH} . \tag{8}$$

This result coinsides with the one derived by using the correlated Einstein model [7] which is considered and used widly [8-18].

The above results are the harmonic potential increases due to replacing the *H* atoms from number 1 to 9 by the *D* atoms ($n \leq 9$). In the case of more increase of *D* atoms in the surface (001) we suppose that the 10th *D* atom is located at the place *B*, the 11th *D* atom at the place *A*, the 12th and 13th *D* atoms at the remaining places. As it has been noted at the beginning, the contributions to the potential increase of the last two are unsignificant that is why it is not important that they are the *D* or the *H* atoms. Now we consider some concret cases:

For $n = 10$, then $n_1 = n_2 = 4$:

$$\begin{aligned} V_{tot} &= \frac{1}{2}K_{\text{eff}}X^2 = 2K_{\text{eff}}X_D^2 \\ &= \frac{1}{2}K_{HD}X_D^2 + \frac{1}{2}K_{DD}4X_D^2 + \frac{1}{2}K_{HD}X_D^2 + K_{DD}X_D^2 + \frac{1}{2}K_{DD}X_D^2 + \frac{1}{2}K_{HD}X_D^2 \\ &= \frac{7K_{DD}+3K_{HD}}{2}X_D^2 \Rightarrow K_{\text{eff}} = \frac{7K_{DD}+3K_{HD}}{4} \end{aligned} \tag{9}$$

For $n = 11, 12, 13$:

$$\begin{aligned} V_{tot} &= \frac{1}{2}K_{DD}X_D^2 + \frac{1}{2}K_{DD}4X_D^2 + \frac{1}{2}K_{HD}X_D^2 + K_{DD}X_D^2 + \frac{1}{2}K_{DD}X_D^2 + \frac{1}{2}K_{HD}X_D^2 \\ &= (4K_{DD} + K_{HD})X_D^2 \Rightarrow K_{\text{eff}} = \frac{4K_{DD}+K_{HD}}{2} \end{aligned} \tag{10}$$

From (7, 8, 10) we obtain

$$\begin{aligned} K_{\text{eff}} &= \frac{5}{2}\delta_{0n}K_{HH} + \delta_{10n}\frac{7K_{DD}+3K_{HD}}{4} + (\delta_{11n}+\delta_{12n}+\delta_{13n})\frac{4K_{DD}+K_{HD}}{2} \\ &+ \frac{1-\delta_{0n}-\delta_{10n}-\delta_{11n}-\delta_{12n}-\delta_{13n}}{4(\varepsilon+1)^2}\begin{Bmatrix} (12-n_1)\varepsilon^2K_{HH} + (n-1)K_{DD} + \\ + [4(\varepsilon+1)^2 + n_1\varepsilon^2 + 13 - n]K_{DD} \end{Bmatrix} \end{aligned} \tag{11}$$

Using this expression we can calculate the effective force constant K_{eff} with different number of impurity atoms replacing the neighboring *H* atoms of the D_0 atom located at the centre of the fcc lattice.

Applying the Morse potential in the approximation for weak anharmonicity by the expansion

$$V(x) = D\left(e^{-2\alpha x} - 2e^{-\alpha x}\right) \cong D\left(-1 + \alpha^2x^2 - \alpha^3x^3 + \cdots\right) \tag{12}$$

for each atomic pair or its form by using the definition [7] $y = x - a$ as the deviation from the equilibrium value x at temperature T, where $a = \langle x \rangle$, $x = r - r_o$, r is instantanious bond length, and r_o is its equilibrium value

$$V(y) = D\alpha^2(1-3\alpha a)y^2 - D\alpha^3y^3 + D\alpha^2(2-3\alpha a)ay + D\alpha^2a^2(1-\alpha.a) - D \tag{13}$$

we obtain the following single-bond spring constants

$$K_{HH} = 2D_H\alpha_H^2\left(1 - 3\alpha_H\langle X_H\rangle\right) = 2D_H\alpha_H^2\left[1 - \frac{3}{2}\delta_{0n}\alpha_H a - \left(1 - \delta_{0n}\right)\alpha_H\frac{3\varepsilon.a}{1+\varepsilon}\right], \quad (14)$$

$$\begin{aligned} K_{DD} &= 2D_D\alpha_D^2\left(1 - 3\alpha_D\langle X_D\rangle\right) \\ &= 2D_D\alpha_D^2\left[1 - \frac{3}{2}(\delta_{10n} + \delta_{11n} + \delta_{12n} + \delta_{13n})\alpha_D a - \left(1 - \delta_{13n} - \delta_{10n} - \delta_{11n} - \delta_{12n}\right)\alpha_D\frac{3a}{1+\varepsilon}\right], \end{aligned} \quad (15)$$

$$K_{HD} = 2D_{HD}\alpha_{HD}^2(1 - 3\alpha_{HD}\langle X_{HD}\rangle) \approx 2D_{HD}\alpha_{HD}^2\left(1 - 3\alpha_{HD}\cdot\frac{a}{2}\right) \quad (16)$$

and the Morse potential parameters D_{HD}, α_{HD} for the case with impurity can be obtained by averaging those of the host atoms D_H, α_H and of the dopant atoms D_D, α_D, where

$$D_{HD} = \frac{D_H + D_D}{2}; \ \alpha_{HD}^2 = \frac{D_H\alpha_H^2 + D_D\alpha_D^2}{D_H + D_D}; \ \alpha_{HD}^3 = \frac{D_H\alpha_H^3 + D_D\alpha_D^3}{D_H + D_D}. \quad (17)$$

Substituting the values of (14-16) into (11) we obtain the effective spring constant

$$\begin{aligned} K_{\text{eff}} &= 5\delta_{0n}D_H\alpha_H^2\left(1 - \frac{3}{2}\alpha_H a\right) + \frac{\delta_{10n}}{2}\left[7D_D\alpha_D^2\left(1 - \frac{3}{2}\alpha_D a\right) + 3D_{HD}\alpha_{HD}^2\left(1 - \frac{3}{2}\alpha_{HD}a\right)\right] \\ &\quad + (\delta_{11n} + \delta_{12n} + \delta_{13n})\left[4D_D\alpha_D^2\left(1 - \frac{3}{2}\alpha_D a\right) + D_{HD}\alpha_{HD}^2\left(1 - \frac{3}{2}\alpha_{HD}a\right)\right] \\ &\quad + \frac{1 - \delta_{0n} - \delta_{10n} - \delta_{11n} - \delta_{12n} - \delta_{13n}}{2(\varepsilon+1)^2} \\ &\quad \left\{\begin{aligned} &(12 - n_1)\varepsilon^2 D_H{\alpha_H}^2\left(1 - \frac{3\varepsilon\alpha_H a}{\varepsilon+1}\right) + (n-1)D_D\alpha_D^2\left(1 - \frac{3\alpha_D a}{\varepsilon+1}\right) + \\ &+ [4(\varepsilon+1)^2 + n_1\varepsilon^2 + 13 - n]D_{HD}\alpha_{HD}^2\left(1 - \frac{3}{2}\alpha_{HD}a\right) \end{aligned}\right\} \end{aligned} \quad (18)$$

Now we test the case when there is not any impurity atom, i.e., $n = 0$, we obtain:

$$\left(K_{H\_\text{pure}}\right)_{EFF} = 5D_H{\alpha_H}^2\left(1 - \frac{3}{2}\alpha_H a\right) \quad (19)$$

This result coinsides totally with the one derived by using the anharmonic correlated Einstein model [7]. From Eq. (13) we obtain the harmonic term

$$V_h(y) = \frac{1}{2}\left\{2D\alpha^2(1 - 3\alpha.a)\right\}y^2 = \frac{1}{2}K_h y^2, \ K_h = 2D\alpha^2(1 - 3\alpha.a) \quad (20)$$

or for different cases

$$V_{HD}(y)=\frac{1}{2}K_{HD}y^2,\ V_{HH}(y)=\frac{1}{2}K_{HH}y^2,\ V_{DD}(y)=\frac{1}{2}K_{DD}y^2 \tag{21}$$

and the anharmonic term of the interaction potential is given by

$$V_{anh}(y)=K_3y^3,\quad K_3=-D\alpha^3. \tag{22}$$

Since this term is cubic power of the parameter y we can use an expression similar to Eq. (5), for the cases $n = 1 \div 9$

$$\begin{aligned}V_{3tot} &= K_{3HD}X_D^{\ 3}+K_{3HD}(X_H+X_D)^3+K_{3HH}X_H^{\ 3}\\ &+n_1K_{3DD}\left(\frac{X_D}{2}\right)^3+n_2K_{3DD}\left(\frac{-X_D}{2}\right)^3+(4-n_1)K_{3HD}\left(\frac{X_D}{2}\right)^3+(4-n_2)K_{3HD}\left(\frac{-X_D}{2}\right)^3\\ &+n_1K_{3HD}\left(\frac{X_H}{2}\right)^3+(4-n_1)K_{3HH}\left(\frac{X_H}{2}\right)^3+4.K_{3HH}\left(\frac{-X_H}{2}\right)^3\end{aligned}$$

and from this we deduce

$$K_{3\mathrm{eff}}(\varepsilon+1)^3=K_{3HD}+K_{3HD}(\varepsilon+1)^3+\varepsilon^3K_{3HH}+\frac{n_1-n_2}{8}(K_{3DD}-K_{3HD})+\frac{n_1\varepsilon^3}{8}(K_{3HD}-K_{3HH})$$

$$\Rightarrow K_{3\mathrm{eff}}=\frac{1}{8(\varepsilon+1)^3}\left\{(8-n_1)\varepsilon^3K_{3HH}+(n_1-n_2)K_{3DD}+[8(\varepsilon+1)^3+n_1\varepsilon^3+8+n_2-n_1]K_{3HD}\right\};$$

$$K_{3\mathrm{eff}}=\frac{-1}{8(\varepsilon+1)^3}\left\{(8-n_1)\varepsilon^3D_H\alpha_H^3+(n_1-n_2)D_D\alpha_D^3+[8(\varepsilon+1)^3+n_1\varepsilon^3+8+n_2-n_1]D_{HD}\alpha_{HD}^3\right\}$$

For the case $n = 10$ we obtain $K_{3\mathrm{eff}}=-\dfrac{17D_D\alpha_D^3+3D_{HD}\alpha_{HD}^3}{16}$,

and for $n = 11, 12, 13$ it is given $K_{3\mathrm{eff}}=-\dfrac{19D_D\alpha_D^3+D_{HD}\alpha_{HD}^3}{16}$.

At the end we obtain

$$\begin{aligned}K_{3\mathrm{eff}} &= -\frac{(1-\delta_{0n}-\delta_{10n}-\delta_{11n}-\delta_{12n}-\delta_{13n})}{8(\varepsilon+1)^3}\left\{\begin{matrix}(8-n_1)\varepsilon^3D_H\alpha_H^3+(n_1-n_2)D_D\alpha_D^3\\ +[8(\varepsilon+1)^3+n_1\varepsilon^3+8+n_2-n_1]D_{HD}\alpha_{HD}^3\end{matrix}\right\}-\\ &-\delta_{10n}\frac{17D_D\alpha_D^3+3D_{HD}\alpha_{HD}^3}{16}-(\delta_{11n}+\delta_{12n}+\delta_{13n})\frac{19D_D\alpha_D^3+D_{HD}\alpha_{HD}^3}{16}-\frac{5}{4}\delta_{0n}D_H\alpha_H^3\end{aligned} \tag{23}$$

which for $n=0$ (without impurity) is reduced to the result derived by using the anharmonic correlated Einstein model [7]

$$K_{3\mathrm{eff}-H} = -\frac{5}{4} D_H \alpha_H^{\ 3} . \tag{24}$$

The remaining anharmonic contribution taken from Eq. (15) is given by

$$D\alpha^2 (2 - 3a\alpha) ay \approx 2D\alpha^2 ay \Rightarrow K_{2a} = 2D\alpha^2 , \tag{25}$$

which contains $2D\alpha^2$. Based on the similarity between K_{2a} of Eq. (25) and K_h of Eq. (20) we can use Eq. (18) to deduce

$$\begin{aligned} K_{2\mathrm{eff}} &= 5\delta_{0n} D_H \alpha_H^2 + \frac{\delta_{10n}}{2}\left[7D_D\alpha_D^2 + 3D_{HD}\alpha_{HD}^2\right] + (\delta_{11n} + \delta_{12n} + \delta_{13n})\left[4D_D\alpha_D^2 + D_{HD}\alpha_{HD}^2\right] \\ &+ \frac{1 - \delta_{0n} - \delta_{10n} - \delta_{11n} - \delta_{12n} - \delta_{13n}}{2(\varepsilon+1)^2}\left\{ \begin{matrix} (12 - n_1)\varepsilon^2 D_H \alpha_H^2 + (n-1) D_D \alpha_D^2 + \\ + [4(\varepsilon+1)^2 + n_1\varepsilon^2 + 13 - n] D_{HD}\alpha_{HD}^2 \end{matrix} \right\} \end{aligned} \tag{26}$$

Hence, the total anharmonic contribution to the atomic interaction potential must be given by

$$V_{\mathrm{anh}}(y) = K_{2\mathrm{eff}}\, ay + K_{3\mathrm{eff}}\, y^3 . \tag{27}$$

For the case $n = 0$, i., e., there is not any dopant atom, from Eqs. (26, 28, 30) we obtain

$$V_{\mathrm{eff}}(y) = \frac{1}{2} K_{EFF}\, y^2 + V_{\mathrm{anh}}(y), \tag{28}$$

$$K_{EFF} = 5D\alpha^2\left(1 - \frac{3}{2}\alpha a\right), \quad V_{\mathrm{anh}}(y) = 5D\alpha^2 ay - \frac{3}{2} D\alpha^3 y^3 . \tag{29}$$

These results coinside with those derived by using anharmonic correlated Einstein model [7] which is considered and used widly in XAFS theory for the pure materials [8-18] providing good agreement with experiment even for Cu with strong anharmonic contributions.

3. Numerical results and discussions

Now we apply the above derived expressions to numerical calculations for fcc crystal Ni doped by several Cu atoms. We calculated the Morse potential of Ni and Cu by using the procedure presented in [19, 21]. The results are illustrated in Figure 3 showing very good agreement with experiment [15] for the case of Ni.

Using these calculated Morse potentials we calculated single-bond and effective spring constants for pure Ni and for Ni doped by several impurity atoms Cu. The results are written in Table I. The effective spring constants are different when Ni is doped by n = 1, 3, 5, 8 Cu atoms.

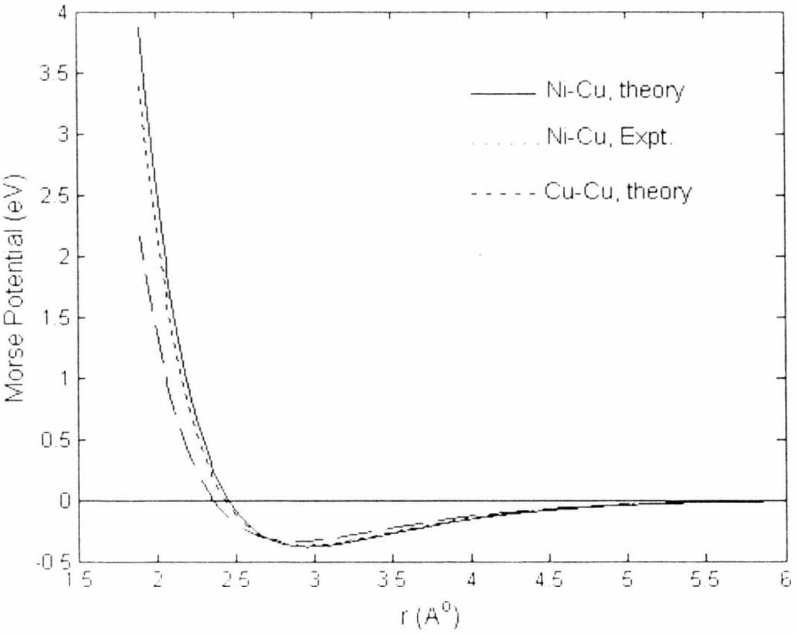


Figure 3. Calculated Morse potential for Ni (solid), Cu (dash), and an comparison to experiment [15] (dot) for the case of Ni.

Table I. Effective spring constants of Ni doped by $n = 0, 1, 3, 5, 8$ Cu atoms and of pure Cu.

N	0	1	3	5	8	*Cu-pure*
K_{eff} $(eV/Å^2)$	4.1757	3.8072	3.7544	3.7016	3.6668	3.1204
$K_{2eff}$$(eV/Å^2)$	4.2389	3.8803	3.8266	3.7728	3.7358	3.1655
$K_{3eff}$$(eV/Å^3)$	-1.5047	-1.3155	-1.3047	-1.2939	-1.3010	-1.0753

Although the values of $K_{2\mathrm{eff}}$ are significant but the term $K_{2\mathrm{eff}}ay$ contains a very small factor a (about 0.007 Å at 300 K), that is why this term contributes not so much to the effective potential. The effective potentials of the system of Ni illustrated in figure 4 calculated by using the effective sping constants of Table I are quite different from the pair potential of Ni shown in figure 3 denoting the importance of the constructed effective potential of the system. Figure 4 also shows significant changes of the effective potential of Ni when it is doped by the impurity Cu atoms. The greater the number of dopant atom Cu is, the bigger the change of the effective potential. The above properties considered for one cluster can be deduced for the whole crystal. These changes will influence on the thermodynamic parameters of the crystals like on the cumulants studied in the XAFS spectroscopy [7, 8, 11, 13, 19].

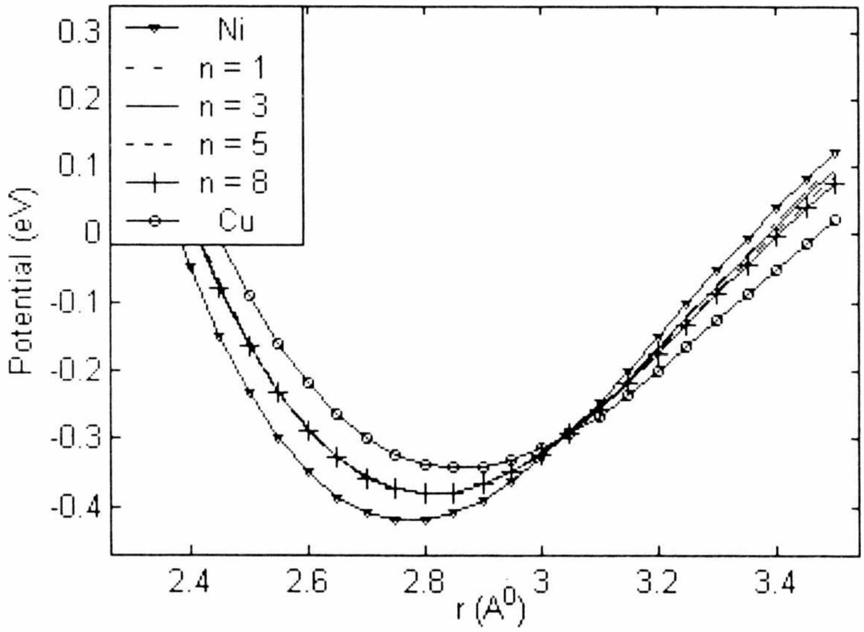


Figure 4. Effective potential of pure Ni and of Ni doped by 0, 1, 3, 5, 8 Cu atoms and of pure Cu.

4. Conclusions

This work has developed a new procedure for description and calculation of the effective potential, single-bond and effective spring constants including anharmonic contributions of a crystal doped by an arbitrary number *n* of impurity atoms.

Derived expressions of the considered quantities approach those derived by using the anharmonic correlated Einstein model for the pure materials which provides very good agreement with the experiment and is used widly [7-18].

This work also denotes the importance of the effective potential of a system and its relation with the pair potential, which is especially important for the XAFS theory [7, 8, 11, 13, 19].

The above properties considered for one cluster can be deduced for the whole crystal so that from this procedure one can deduce a method for description and calculation of the atomic interaction effective potential and force constants of an alloy consisting of different percentage of constituent elements.

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References

1. R. B. Greegor, F. W. Lytle, *Phys. Rev.* B**14**(1979) 4902.
2. J. M. Tranquada, R. Ingalls, *Phys. Rev.* B**28**(1983) 3520.
3. E. A. Stern, P. Livins, Zhe Zhang, *Phys. Rev.* B**43**(1991) 8850.
4. N. V. Hung, R. Frahm, *Physica* B **208** & **209**(1995) 91.
5. N. V. Hung, R. Frahm, H. Kamitsubo, *J. Phys. Soc. Jpn.* **65**(1996) 3571.
6. N. V. Hung, *J. de Physique* **IV**(1997) C2 : 279.
7. N. V. Hung, J. J. Rehr, *Phys. Rev.* B**56**(1997) 43.
8. N. V. Hung, N. B. Duc, R. R. Frahm, *J. Phys. Soc. Jpn.* **72**(2003) 1254.
9. T. Yokoyama, *Phys. Rev.* B**57**(1998) 3423.
10. A.V. Poiarkova, J. J. Rehr, *Phys. Rev.* B**59**(1999) 948.
11. J. J. Rehr, R. C. Albers, *Rewiews of Modern Physics*, Vol. **72**(2000) 621.
12. T. I. Nedoseikina, A. T. Shuvaev, V. G. Vlasenko, *J. Phys.: Condens. Matter* **12**(2000) 2877.
13. P. Fornasini, F. Monti, A. Sanson, *J. Synchrotron Radiation* **8**(2001) 1214.
14. Y. Okamoto, M. Akabori, H. Motohashi, H. Shiwaku, T. Ogawa, *J. Synchrotron Radiation*, Vol. **8**(2001) 1191.
15. I. V. Pirog, T. I. Nedoseikina, I. A. Zarubin, A. T. Shuvaev, *J. Phys.: Condens. Matter* **14**(2002) 1825.
16. I. V. Pirog, T. I. Nedoseikina, *Physica* B**334**(2003) 123.
17. N. V. Hung, *VNU-Jour. Science,* Vol. **18**, No. 3(2002) 17.
18. N. V. Hung, D. X. Viet, *VNU-Jour. Science* Vol. **19**, No. 2(2003) 19.
19. M. Daniel, D. M. Pease, N. V. Hung, J. I. Budnick, *in press in Phys. Rev.* B (2003).
20. N. V. Hung, *VNU-Jour. Science*, Vol. **19**, No. 4 (2003) 19.