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Möbius transform and inversion from cohesion to elastic constants

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Abstract. Elastic constants have been calculated for the FCC metals Cu, Al and Ni using the Möbius transform and a short-range three-body potential correction. Unlike a previous calculation based only on pair potentials, the present result is in good agreement with experiment since the restriction of the Cauchy relation has been removed. More importantly, it shows the potential application of the Möbius-inversion method for evaluating interatomic potentials from *ab initio* electronic structure calculations.

1. Introduction

Recently, the obscure Möbius inversion formula in number theory has been applied to different kinds of inverse problems in physics [1–12]. In particular, the Möbius formula for lattice problems can be used to obtain pair potentials for FCC and BCC metals from cohesive energy calculations [7, 11]. The inversion is exact for radial pair potentials with much faster convergence than the earlier reported method of Carlsson and co-workers [13]. In this paper, the Möbius-inverted pair potential is used to calculate the elastic constants of FCC transition metals by including the corrections for the short-range three-body interactions. The calculated results are in good agreement with experiment, and the Cauchy relation between the elastic constants has been removed completely.

2. Formalism

In general, the binding energy per atom might be expressed as

$$E(r) = \frac{(1/N)}{2!} \sum'_{i,j} \phi^{(2)}(r_{ij}) + \frac{(1/N)}{3!} \sum'_{i,j,k} \phi^{(3)}(r_{ij}, r_{jk}, r_{ki}) + \dots \quad (1)$$

where r represents the lattice constants, $\phi^{(2)}$ and $\phi^{(3)}$ are the two-body and three-body interatomic potentials respectively, r_{ij} is the displacement vector from the i th atom to the j th atom; Σ' represents that the zero displacement is not included. If we ignore the three-body interactions and all the higher-order multibody interactions, we can obtain the exact formal solution of pair potential from inverting the binding energy curves [6, 7, 11]. Pair potentials are widely used for modelling a variety of mechanical and defect properties, phonon dispersion, and so on. As is well known, calculations based only on pair potentials

leave many shortcomings, such as the Cauchy relation [14], which is due to a many-body effect of electronic origin. Here we consider the simplest correction, namely that of the three-body interaction. If the atom under consideration is at the origin, and we take a simplified form for the three-body interaction, then (1) can be expressed as

$$E(r) = (1/2) \sum_{R_i \neq 0} \phi^{(2)}(\mathbf{R}_i) + \frac{1}{6} \sum_{\substack{R_i \neq R_j \\ R_i, R_j \neq 0}} \phi^{(3)}(\mathbf{R}_i, \mathbf{R}_j). \quad (2)$$

Brunch and McGee [15] have proposed a Slater–Kirkwood-type non-additive three-body energy for dense helium:

$$\phi^{(3)}(\mathbf{R}_i, \mathbf{R}_j) = [e^{-\alpha(R_i+R_j+R_{ij})} + c(R_i R_j R_{ij})^{(-3)}](1 + \cos \theta_1 \cos \theta_2 \cos \theta_3) \quad (3)$$

where θ_1 , θ_2 and θ_3 are the inner angles of triangle formed by \mathbf{R}_i , \mathbf{R}_j and \mathbf{R}_{ij} . The first exponential term of this equation represents the exchange three-body interaction which describes the alterations of the charge densities of two interacting atoms by the presence of a third one at small interatomic distances. The second term, known as the Axilrod–Teller (AT) term, represents the triple-dipole interaction which is the dominant contribution of the three-body interactions between atoms with closed shells. In the lower-density region, the Axilrod–Teller three-body interaction is the main part of the three-body energy and leads to an accurate description of dense rare gases, while the three-body exchange interaction is greater in magnitude than the AT term for small interatomic distances [18, 19].

In the present work, we take this short-range three-body potential as the three-body interaction in FCC metals, namely

$$\phi^{(3)}(\mathbf{R}_i, \mathbf{R}_j) = A e^{-\alpha(R_i+R_j+R_{ij})} (1 + \cos \theta_1 \cos \theta_2 \cos \theta_3) \quad (4)$$

where α is the decay constant for the three-body interaction, which is dependent on the particular element. In fact, such an empirical expression for the short-range three-body interaction in a lattice was suggested by Sarkar and Sengupta [20]. The proposed three-body potential leads to some satisfying calculations of the lattice dynamical properties of transition metals [21].

From the physical point of view, the three-body interaction is of short range [22], reflecting the simultaneous overlap of the electronic orbital of the three atoms under consideration. Obviously, it could affect the shear modulus significantly. In the following discussion, we limit the short-range three-body forces in the FCC system up to only second-nearest neighbours due to its short-range property. For first-nearest neighbours, the corresponding R_i and θ_i are given by

$$(R_i, R_j, R_{ij}) = (r/\sqrt{2}, r/\sqrt{2}, r/\sqrt{2}) \quad (5a)$$

$$(\theta_1, \theta_2, \theta_3) = (\pi/3, \pi/3, \pi/3) \quad (5b)$$

where r is the lattice constant. Inducing second-nearest neighbours, the corresponding R_i and θ_i are given by

$$(R_i, R_j, R_{ij}) = (r/\sqrt{2}, r, r/\sqrt{2}) \quad (6a)$$

$$(\theta_1, \theta_2, \theta_3) = (\pi/4, \pi/2, \pi/4). \quad (6b)$$

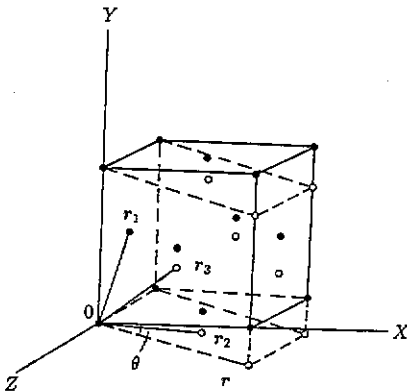


Figure 1. The calculation of sheared three-body energy: consider the (100) plane sheared along the (010) direction.

Consequently, the contribution to the binding energy of an unsheared FCC lattice from the three-body potential is given by

$$\frac{1}{6} \sum \phi^{(3)} = \frac{24}{6} A e^{-(3\sqrt{2}/2)ar} (1 + \frac{1}{8}) + \frac{24}{6} A e^{-(1+\sqrt{2})ar} = 4.5 A e^{-(3\sqrt{2}/2)ar} + 4 A e^{-(1+\sqrt{2})ar} \tag{7}$$

For evaluating the decay constant α we assume that if one of R_i, R_j, R_{ij} is equal to the next-neighbor distance, then the corresponding three-body interaction becomes negligible, i.e.

$$\frac{e^{-(1+\sqrt{2})ar}}{e^{-(3\sqrt{2}/2)ar}} = \frac{e^{-ar}}{e^{-ar/\sqrt{2}}} \leq 10^{-n} \tag{8}$$

To evaluate the elastic constants, we will calculate the deformation energy for small strains about the equilibrium. If ϵ is the strain for a stretching deformation, then the lattice constant r along the direction of stretching is

$$r = a_0(1 + \epsilon) \tag{9a}$$

where a_0 is the equilibrium lattice constant. For a shear deformation, as in figure 1, the corresponding lattice constant is

$$r = a_0\sqrt{1 + \epsilon^2} \cong a_0(1 + \epsilon^2/2) \tag{9b}$$

Therefore, for determining α in our calculation, we substitute the equilibrium lattice constant a_0 into (8), and define a material independent parameter β as

$$\beta = \alpha a_0 \tag{10}$$

such that

$$\beta \geq \frac{n \text{Ln}10}{1 - 1/\sqrt{2}} = 7.8615173n \tag{11}$$

We take $n = 0.5$ so that

$$\beta = 3.9307587 \tag{12}$$

For each particular element, we adjust the parameter β (or n) around 3.9, until satisfactory results for elastic constants are obtained.

Now let us consider the pair potentials. We denote $E^{(2)}(r)$ as follows:

$$E^{(2)}(r) = E(r) - 4.5Ae^{-(3\sqrt{2}/2)\alpha r} - 4Ae^{-(1+\sqrt{2})\alpha r} \quad (13)$$

where $E^{(2)}(r)$ represents the contribution to the binding energy from the pair potentials. For the FCC lattice we can write $E^{(2)}(r)$ in the following way:

$$\begin{aligned} E^{(2)} &= \left(\frac{1}{2}\right) \sum_{|\mathbf{R}_i| \neq 0} \phi^{(2)}(|\mathbf{R}_i|) \\ &= 3 \sum_{s=1}^{\infty} \phi^{(2)}(sr) + 6 \sum_{s,t=1}^{\infty} [\phi^{(2)}\{(s^2+t^2)r\}^{1/2} + \phi^{(2)}\{(s-\frac{1}{2})^2 + (t-\frac{1}{2})^2\}r] \\ &\quad + 4 \sum_{s,u,t=1}^{\infty} [\phi^{(2)}\{(s^2+t^2+u^2)r\}^{1/2} + 3\phi^{(2)}\{(s-\frac{1}{2})^2 + (t-\frac{1}{2})^2 + u^2\}r]. \end{aligned} \quad (14)$$

Here, $\phi^{(2)}$ is the pair potential, the first sum coming from the points lying along the axes. The six different directions give a weight of $6/2 = 3$. The first term of the second sum arises from the points on the cube edges lying on the coordinate planes, while the second expression arises from the points on this plane that lie on the face centres. Each of these contributions have a weight of $12/2 = 6$. The first expression in the last sum arises from the points on the cube edges away from the coordinate planes. Each carries its appropriate weight. Equation (14) is exact.

We now use the modified Möbius inversion for the lattice [6,7] to calculate the pair potential from (14) with very fast convergence. We introduce an operator \mathcal{G} to rewrite the first sum, and the $s = t$ terms in the second sum in (14), as

$$\mathcal{G}\phi(r) = \sum_{s=1}^{\infty} 6[\phi(sr/\sqrt{2}) + (\frac{1}{2})\phi(sr)]. \quad (15)$$

The remaining part of the right-hand side of (14) can be expressed as

$$\begin{aligned} \mathcal{R}\phi(r) &= 6 \sum_{s,t=1}^{\infty} [\phi\{(s^2+t^2)r\}^{1/2} + \phi\{(s-\frac{1}{2})^2 + (t-\frac{1}{2})^2\}r] \\ &\quad + 4 \sum_{s,u,t=1}^{\infty} [\phi\{(s^2+t^2+u^2)r\}^{1/2} + 3\phi\{(s-\frac{1}{2})^2 + (t-\frac{1}{2})^2 + u^2\}r] \end{aligned} \quad (16)$$

with another operator \mathcal{R} , where \sum' means that the sum does not include the terms of $s = t$.

Introduce an operator \mathcal{N} such that

$$\mathcal{N}f(r) = \frac{1}{8} \sum_{m,n=1}^{\infty} (-1/2)^{m-1} (\mu)(n) f(2^{m/2}nr) \quad (17)$$

where $\mu(n)$ is the Möbius function defined by

$$\mu(n) = \begin{cases} 1 & \text{if } n = 1 \\ (-1)^q & \text{if } n \subset p(q) \\ 0 & \text{otherwise.} \end{cases} \quad (18)$$

Here $n \subset P(q)$ means that n is a product of q distinct prime numbers. Then

$$\begin{aligned} \mathcal{N}\mathcal{G}\phi(r) &= \mathcal{N} \sum_{s=1}^{\infty} 6[\phi(sr/\sqrt{2}) + \frac{1}{2}\phi(sr)] \\ &= \sum_{m,n,s=1}^{\infty} [(-1)^{m-1}(1/2)^{m-1}\mu(n)\phi(2^{(m-1)/2}nsr) \\ &\quad + (-1)^{m-1}(1/2)^m\mu(n)\phi(2^{m-2}nsr)]. \end{aligned} \tag{19}$$

If we change the dummy variable in the first expression from m to $m' = m - 1$ then we note that, except for the terms for $m' = 0$, every other term exactly cancels with a corresponding term in the second expression. Thus we finally have

$$\mathcal{N}\mathcal{G}\phi(r) = \sum_{n,s=1}^{\infty} \mu(n)\phi(snr). \tag{20}$$

By using the Möbius inversion theorem [16] which states that if

$$F(r) = \sum_{n=1}^{\infty} f(nr) \tag{21a}$$

then

$$f(r) = \sum_{n=1}^{\infty} \mu(n)F(nr) \tag{21b}$$

and vice versa, it immediately follows that

$$\mathcal{N} = \mathcal{G}^{-1}. \tag{22}$$

Equation (14) becomes

$$E^{(2)}(r) = (\mathcal{G} + \mathcal{R})\phi^{(2)}(r) \tag{23}$$

therefore

$$\begin{aligned} \phi^{(2)}(r) &= (1 + \mathcal{G}^{-1}\mathcal{R})^{-1}\mathcal{G}^{-1}E^{(2)}(r) = (1 + \mathcal{N}\mathcal{R})^{-1}\mathcal{N}E^{(2)}(r) \\ &= (1 - \mathcal{N}\mathcal{R} + \mathcal{N}\mathcal{R}\mathcal{N}\mathcal{R} - \dots)\mathcal{N}E^{(2)}(r) \\ &= (\mathcal{N} - \mathcal{N}\mathcal{R}\mathcal{N} + \mathcal{N}\mathcal{R}\mathcal{N}\mathcal{R}\mathcal{N} - \dots)E^{(2)}(r). \end{aligned} \tag{24}$$

From (15), (22) and (24) one can see that the zero-order approximation

$$\phi^{(2)}(r) = \mathcal{N}E^{(2)}r \tag{25}$$

has already included all the atoms in both the most close-packed and the second-most close-packed directions. This approach is different from most treatments in solid state physics, which only cover nearest- and second-nearest neighbour atoms.

The reason why the present procedure is much faster than the previous work by Carlsson and co-workers [13] arise from the cancellation in this modified Möbius method [6].

Table 1. The calculated binding energy for Cu. $\sigma = (a_0/a)^3$ (a_0 is the equilibrium lattice constant).

σ	0.5	0.7	0.9	1.0	1.5	2.0
E_c (eV/atom)	-2.54	-3.02	-3.55	-3.62	-3.60	-2.05
a (Å)	4.548	4.066	3.739	3.61	3.154	2.865

The binding energy in (2) can be obtained by performing an LMTO calculation [23]. Taking the calculation for copper as an example, the binding energy calculation based on the LMTO method proceeds in 1/48 of the volume of the first Brillouin zone with 89 k -points. The $4s^1 3d^{10}$ electrons are considered as the valence electrons for the atomic configuration. Table 1 gives the binding energy calculated for various lattice constants.

The binding energy curves for Cu, Al and Ni, which have been calculated by the above method, are fitted as follows.

(i) The fitting curve of the binding energy for Cu is

$$E(r) = 3.663855(1.281748 \times 10^3 e^{-1.988682r} - 71.60301e^{-0.994341r}) \quad r \geq 2.4 \text{ \AA} \quad (26)$$

$$E(r) = 11.744916(2.205357 \times 10^3 e^{-2.779431r} - 3.598352/r - 0.099986) \quad r < 2.4 \text{ \AA} \quad (27)$$

(ii) The formula for Al is

$$E(r) = 3.507(6.50174 \times 10^2 e^{-1.60987r} - 50.99702e^{-0.80494r}) \quad r \geq 2.4 \text{ \AA} \quad (28)$$

$$E(r) = 11.499605(5.38165 \times 10^2 e^{-2.0926r} - 4.02345/r) \quad r < 2.4 \text{ \AA} \quad (29)$$

(iii) The formula for Ni is

$$E(r) = 4.43611(8.09163 \times 10^2 e^{-1.91224r} - 56.89157e^{-0.95612}) \quad r \geq 2.4 \text{ \AA} \quad (30)$$

$$E(r) = 9.31416(2.52495 \times 10^4 e^{-3.62009r} - 3.50165/r) \quad r < 2.4 \text{ \AA}. \quad (31)$$

Here, the binding energy is in eV per atom, and the lattice constant is in Å.

The general shape of our binding energy for Cu is quite close to that of [13], but differs a little more from that of [7], especially for the repulsive part. For the value of binding energy at equilibrium, our result is close to the experimental data, the result of [13] being much deeper than ours.

3. Calculated elastic constants

If the three-body contribution is neglected (i.e. $A = 0$), then the corresponding pair potentials may be obtained directly from the Möbius inversion. They are plotted in figure 2. We have fitted these curves by the following analytic expressions.

(i) For Cu

$$\phi(r) = 0.3593792(e^{-2.778302(r-2.857)} - 2e^{-1.389151(r-2.587)}). \quad (32)$$

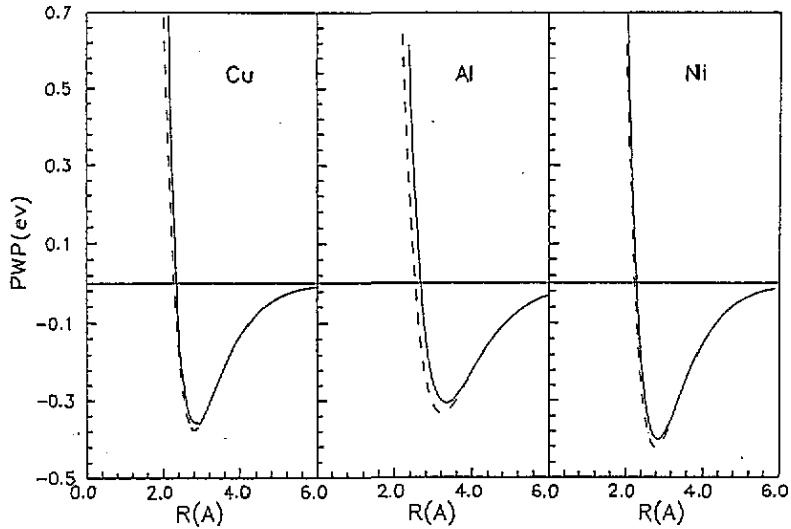


Figure 2. The pair potentials of Cu, Al and Ni as a function of distance between atoms. Full curve: the three-body interactions are free. Broken curve: consider the correction of three-body potential by taking $A = 10^4$ and $n = 0.72$ for Cu, $A = 5.89 \times 10^2$ and $n = 0.51$ for Al, $A = 7.94 \times 10^2$ and $n = 0.6$ for Ni.

(ii) For Al

$$\phi(r) = 0.306135(e^{-2.238012(r-3.323)} - 2e^{-1.119006(r-3.323)}). \quad (33)$$

(iii) For Ni

$$\phi(r) = 0.403067(e^{-2.663244(r-2.852)} - 2e^{-1.331622(r-2.852)}). \quad (34)$$

The calculated elastic constants are compared with the experimental data in table 2 (see the three lines designated '2 - b only'). Obviously, the Cauchy relation

$$C_{12} = C_{44} \quad (35)$$

holds. This result is the same as that of any spherical pair potential model and contrary to experiment, especially Cu and Al.

The three-body interaction $E^{(3)}$ is now included so that $A \neq 0$. For copper, as an example, if A is taken as 10^4 eV and $n = 0.72$ (see table 2), then $E^{(3)} \cong (8.76 \times 10^{-2})E$. Therefore the pair potential is changed to

$$\phi(r) = 0.3712595(e^{-2.730804(r-2.814)} - 2e^{-1.365402(r-2.814)}). \quad (36)$$

The corresponding binding energy $E^{(3)}$ under the shear shown in figure 1 can be expressed as

$$\begin{aligned} E^{(3)}(r) = & \frac{3}{16}A(4e^{-\alpha r_1 - \alpha r_2 - \alpha|r_1 - r_2|} + 4e^{-\alpha r_2 - \alpha r_3 - \alpha|r_2 - r_3|} \\ & + 4e^{-\alpha r_1 - \alpha r_3 - \alpha|r_1 - r_3|} + 4e^{-\alpha r'_1 - \alpha r'_2 - \alpha|r'_1 - r'_2|} \\ & + 4e^{-\alpha r'_2 - \alpha r'_3 - \alpha|r'_2 - r'_3|} + 4e^{-\alpha r'_1 - \alpha r'_3 - \alpha|r'_1 - r'_3|}) \\ & + \frac{2}{3}A(2e^{-\alpha(1+\sqrt{2})a_0} + e^{-\alpha r - \alpha r_3 - \alpha|r - r_3|} \\ & + e^{-\alpha a_0 - \alpha r_3 - \alpha|r - r_3|} + e^{-\alpha r - 2\alpha r_2} + e^{-\alpha a_0 - 2\alpha r_2}) \end{aligned} \quad (37)$$

Table 2. Comparison of the calculated and experimental elastic constants in units of 10^{11} Pa; B is the bulk modulus. In this calculation with the corrections of three-body interactions, the parameters have been taken as follows: $A = 10^4$, $n = 0.72$ for Cu; $A = 5.89 \times 10^2$, $n = 0.51$ for Al and $A = 7.94 \times 10^2$, $n = 0.6$ for Ni. A is in eV and n is dimensionless.

		C_{11}	C_{12}	C_{44}	C_{12}/C_{44}	B
Cu	Experiment [17]	1.762	1.249	0.818	1.527	1.420
	Carlsson <i>et al</i> [13]	2.050	1.400	—	—	1.650
	Present 2 - b only	1.775	1.262	1.270	0.994	1.432
	Present 3 - b includ.	1.741	1.278	0.802	1.594	1.432
Al	Experiment [17]	1.143	0.619	0.316	1.958	0.794
	Present 2 - b only	1.051	0.678	0.668	1.015	0.803
	Present 3 - b includ.	1.179	0.615	0.409	1.504	0.803
Ni	Experiment [17]	2.612	1.508	1.317	1.145	1.876
	Present 2 - b only	1.996	1.488	1.493	0.997	1.647
	Present 3 - b includ.	2.091	1.425	1.315	1.084	1.647

where

$$r'_i \Rightarrow r_i \quad i = 1, 2, 3 \quad (38a)$$

and

$$\theta' \Rightarrow -\theta. \quad (38b)$$

From figure 1, we find

$$r_1 = |r_2 - r_3| = a_0/\sqrt{2} \quad (39)$$

$$r_2 = |r_3 - r_1| = a_0/2\sqrt{2 + \tan^2 \theta} \cong (a_0/\sqrt{2})(1 + \theta^2/4) \quad (40)$$

$$r_3 = (a_0/2)\sqrt{1 + (1 - \tan \theta)^2} \cong (a_0/\sqrt{2})(1 - \theta/2) \quad (41)$$

$$|r_1 - r_2| = |r - r_3| = (a_0/2)\sqrt{1 + (1 + \tan \theta)^2} \cong (a_0/\sqrt{2})(1 + \theta/2) \quad (42)$$

and

$$r = a_0\sqrt{1 + \tan^2 \theta} \cong a_0(1 + \theta^2/2) \quad (43)$$

where a_0 is the equilibrium lattice constant and $\varepsilon = \tan \theta$ is the shearing strain. Therefore, the corresponding results of the calculated elastic constants are shown in table 2 (see the three lines designated by '3 - b includ.'). By using the three-body interaction correction, the results are in excellent agreement with experimental data. Also, the Cauchy relation has been violated, as the experiment requires.

4. Discussion and conclusion

The pair and three-body potentials of FCC Cu, Al and Ni have been applied to calculate the elastic constants without the restriction of the Cauchy relation. In this calculation, the parameters of A and α are both adjustable; the corresponding calculated results of elastic

constants are listed in table 3. Within this chosen range of A and α , the results are not particularly sensitive to the input parameters. The three-body interaction can account for the Cauchy experimental discrepancies. For the parameters A and n shown in table 2, which lead to acceptable predicted values, the ratio of $E^{(3)}/E^{\text{tot}}$ is 8.76×10^{-2} , 2.7×10^{-1} and 4.41×10^{-2} for Cu, Al and Ni respectively, so that the pairwise energy contributes to the main part of the total energy. If the ratio $E^{(3)}/E^{\text{tot}}$ is larger than a threshold value R_c , ($R_c \simeq 3 \times 10^{-1}$), then the FCC structure would be unstable to stretching or shearing. This restricts the choice of parameters.

Table 3. Some results of calculated elastic constants as we adjust the parameters A and n .

	$A(10^3 \text{ ev})$	n	C_{11}	C_{12}	C_{44}	C_{12}/C_{44}
Cu	5.01	0.65	1.856	1.220	0.687	1.775
	10	0.7	1.790	1.253	0.688	1.821
	10	0.73	1.714	1.291	0.846	1.526
	10	0.75	1.741	1.278	0.961	1.330
	10	0.8	1.714	1.291	1.069	1.208
	63.1	0.9	1.654	1.321	1.010	1.308
	31.6	1	1.714	1.291	1.146	1.127
Al	0.589	0.49	1.292	0.559	0.312	1.920
	0.569	0.495	1.246	0.582	0.359	1.621
	0.501	0.5	1.191	0.609	0.437	1.394
	0.575	0.5	1.246	0.582	0.363	1.603
	0.562	0.51	1.179	0.615	0.425	1.447
	0.562	0.52	1.144	0.632	0.437	1.446
	0.562	0.54	1.113	0.648	0.539	1.202
Ni	0.1	0.44	2.209	1.366	1.268	1.077
	0.1	0.445	2.186	1.378	1.315	1.048
	0.1	0.45	2.186	1.378	1.345	1.024
	0.1	0.5	2.115	1.413	1.416	1.274
	1	0.6	2.132	1.405	1.350	1.041
	0.316	0.6	2.215	1.363	1.143	1.192

A similar approach has also been applied to calculating the phonon dispersion relations for FCC transition metals [12]. The calculated results are in excellent agreement with the experiment, improving markedly the pair potential predictions. Based on the calculated pair and three-body potentials, the phonon spectra for materials with strain can be evaluated directly. From the above, the potential applications of Möbius method would be very attractive for evaluating the properties of materials.

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