Model-potential study of the lattice dynamics and elastic constants of the $Ni_{0.55}Pd_{0.45}$ alloy

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A first-principles calculation has been done to compute the force constants of fcc Ni and Pd by applying the transition-metal model potential of Animalu. These force constants are derived up to 10 sets of nearest neighbors, and then a real-space analysis is done to study the dynamical behavior and elastic constants of the two *d*-band metals. A linear relation is used to compute the lattice constant of the alloy $Ni_{0.55}Pd_{0.45}$. Next the force constants of the metals are evaluated at this lattice constant of the alloy. The lattice dynamics and elastic constants of the $Ni_{0.55}Pd_{0.45}$ alloy are then computed by using the force constants and mass for the alloy, obtained by the concentration averages of the force constants and masses of the component metals. In each case, the present microscopic real-space analysis gives the phonon dispersion curves and elastic constants reasonably comparable with the available experimental data. Finally a three-body potential is incorporated in the lattice-dynamical calculation and in all cases, the transverse branches are improved. Thus on one hand, the present calculation explains the lattice dynamics and elastic constants of Ni, Pd, and $Ni_{0.55}Pd_{0.45}$ alloy and, on the other, it shows that a mean-crystal model works well for the high-concentration alloy, $Ni_{0.55}Pd_{0.45}$.

I. INTRODUCTION

The lattice dynamics of pure fcc Ni and Pd transition metals has been experimentally studied by Birgeneau *et al.*[1] and Miller and Brockhouse,[2] respectively. Ni and Pd form solid solutions at all concentrations and at 45 at. % Pd, the Ni-Pd system is a random substitutional disordered alloy. The lattice dynamics of $Ni_{0.55}Pd_{0.45}$ high-concentration alloy has been studied by Kamitakahara and Brockhouse[3] by the method of inelastic scattering of neutrons. These authors derive the force constants of Ni and Pd from the phonon dispersion curves in the Born–Von Karman model and, in the mean-crystal model, they obtain a reasonably good fit for the phonon dispersion in the $Ni_{0.55}Pd_{0.45}$ alloy by using as many as 16 force parameters. A similar fit is obtained by Upadhyaya and Shyam.[4] They use a three-body electron-gas phenomenological force model with six constants for component Ni and Pd metals and then evaluate the force constants of the $Ni_{0.55}Pd_{0.45}$ alloy by taking the concentration averages of the force constants of the two metals. In both of these works, the resultant force constants for component metals are obtained by fitting with the experimental data. Since a reliable transition-metal model potential (TMMP) for fcc *d*-band metals due to Animalu[5] is available, we plan to perform a first-principles calculation of the phonon dispersion and elastic constants of fcc Ni, Pd, and $Ni_{0.55}Pd_{0.45}$ metallic systems.

In the present work, the TMMP of Animalu[5] is first used to compute the radial and tangential force constants of fcc Ni and Pd up to 10 sets of nearest neighbors at the experimental lattice constants. These microscopic force constants are then used to compute the phonon dispersion and elastic constants of pure fcc Ni and Pd transition metals in the real-space analysis. In order to study the vibrational and elastic properties of the $Ni_{0.55}Pd_{0.45}$ alloy, the force constants of Ni and Pd are again calculated for the fcc phase at the lattice constant of the alloy. A linear superposition of the force constants and masses of the component metals is used to deduce the averaged force constants and mass of the alloy. The values of the force constants and the mass, so obtained for the $Ni_{0.55}Pd_{0.45}$ alloy, are then fed into the dispersion and elastic relations and computed results are compared with the available experimental data.

It will be seen that, although a reasonably good agreement is obtained for the longitudinal branches, in general, the transverse branches are deviating substantially from the measured data for the component metals as well as for the alloy. In fact, the present model pseudopotential analysis in second order describes the interaction system in the central pairwise form and the contribution due to the third-order terms resulting in the three-body effect may be contributory. In the present procedure, we include the effect of third-order terms in the form of a three-body potential following the work of Upadhyaya and Prakash.[6] The effect of three-body forces is incor-

porated in the computation of phonon dispersion and elastic constants of the component metals as well as those of the alloy. Vibration spectra, specific heat, and Debye temperature are also computed for the $Ni_{0.55}Pd_{0.45}$ alloy by using alloy force constants. Necessary theory for the calculation is presented in Sec. II and the numerical results with discussions are given in Sec. III.

II. THEORY

The normal-mode phonon frequencies (ν) of the fcc system corresponding a wave vector $\mathbf{q}$ can be calculated by solving the secular equation

$$|D(\mathbf{q})-4\pi^2 M\nu^2 I|=0 , \tag{1}$$

where $D(\mathbf{q})$ is the dynamical matrix of the order (3×3), I is the unit matrix, and M is the ionic mass. In the present work, the dynamical matrix elements $D_{\alpha\beta}(\mathbf{q})$ are composed of two-body central pairwise and three-body (many-body) parts:

$$D_{\alpha\beta}(\mathbf{q})=D^{\rm cp}_{\alpha\beta}(\mathbf{q})+D^{m}_{\alpha\beta}(\mathbf{q}) . \tag{2}$$

Pseudopotential theory in second order describes the interatomic interaction in the central pairwise form:[7]

$$\Phi(r)=\frac{Z^2e^2}{r}-\frac{2Z^2e^2}{\pi}\int_0^\infty G(q)\frac{\sin qr}{qr}dq , \tag{3}$$

where Z is the valency, e is the electronic charge, and $G(q)$ is the normalized energy wave-number characteristic given by

$$G(q)=\left[\frac{4\pi Ze^2}{\Omega q^2}\right]^{-2}\frac{V_b(q)^2}{1-f(q)}\left[1-\frac{1}{\epsilon(q)}\right] , \tag{4}$$

where $V_b(q)$ is the bare ion model potential and $\epsilon(q)$ is the dielectric function. Here we use the transition-metal model potential of Animalu[5] in the local approximation with the dielectric function due to Hubbard and Sham. In the case of the central interaction, first and second derivatives of the pair potential provide two independent force constants for a particular set of neighbors:[7]

$$\frac{1}{r}\frac{d\Phi}{dr}=-\frac{Z^2e^2}{r^3}-\frac{2Z^2e^2}{\pi r^2}\int_0^\infty G(q)\left[\cos qr-\frac{\sin qr}{qr}\right]dq \tag{5}$$

and

$$\frac{d^2\Phi}{dr^2}=\frac{2Z^2e^2}{r^3}-\frac{2Z^2e^2}{\pi r}\int_0^\infty G(q)\left[\frac{2\sin qr}{qr^2}-\frac{2\cos qr}{r}-q\sin qr\right]dq . \tag{6}$$

We denote the radial force constant $[d^2\Phi/(dr^2)]_{r_i}=\alpha_i$ and tangential force constant

$$\left[\frac{1}{r}\frac{d\Phi}{dr}\right]_{r_i}=\beta_i$$

for the ith set of neighbors.

Now, if $G(q)$ is known, we can evaluate the radial and tangential force constants for a particular set of nearest neighbors by using Eqs. (5) and (6). In the present work we use the TMMP of Animalu[5] to calculate the force constants of Ni and Pd transition metals. First, the calculation of radial and tangential force constants (α_i and β_i) is done at the lattice parameter of each metal and next the calculation is repeated for each metal at the lattice parameter of the $Ni_{0.55}Pd_{0.45}$ alloy. The lattice constant for the alloy $Ni_{0.55}Pd_{0.45}$ is calculated by using a linear relation

$$a(\text{Ni-Pd})=0.55a(\text{Ni})+0.45a(\text{Pd}) . \tag{7}$$

The force constants, evaluated at the lattice constant of the alloy, are used to evaluate the force constants of the $Ni_{0.55}Pd_{0.45}$ alloy using the linear relation

$$\alpha_i(\text{NiPd})=0.55\alpha_i(\text{Ni})+0.45\alpha_i(\text{Pd}) \tag{8}$$

and

$$\beta_i(\text{NiPd})=0.55\beta_i(\text{Ni})+0.45\beta_i(\text{Pd}) . \tag{9}$$

The concentration average mass, used in the calculation for the alloy, is obtained from the following relation:

$$M(\text{NiPd})=0.55M(\text{Ni})+0.45M(\text{Pd}) . \tag{10}$$

Following Maradudin *et al.*,[8] the consideration of central pairwise forces up to 10 sets of nearest neighbors in the fcc system yields the dynamical matrix elements[9] $D^{\rm cp}_{\alpha\beta}(\mathbf{q})$, involving 20 force parameters $\alpha_i,\beta_i,i=1-10$. In order to compute the contribution of many-body forces to the dynamical matrix elements $D^{m}_{\alpha\beta}(\mathbf{q})$, we follow the scheme of Upadhyaya and Prakash,[7] where a three-body empirical potential is used to deduce the force-constant matrix, involving a single parameter A.

Now one can construct the dynamical matrix $D(\mathbf{q})$ by using Eq. (2) and then solve the secular equation (1) to compute the phonon frequencies (ν) corresponding to a wave vector ($\mathbf{q}$) in the Brillouin zone for a pure transition metal (Ni or Pd) or alloy (Ni-Pd). For the calculation of the elastic constants, we solve the secular equation (1) in the long-wavelength limit ($\mathbf{q}\to0$) up to 10 sets of nearest neighbors and obtain the following relations:

$$\begin{aligned}C_{11}=\frac{1}{a}(&2\alpha_1+2\beta_1+4\alpha_2+12\alpha_3+12\beta_3+8\alpha_4+8\beta_4\\&+\tfrac{164}{5}\alpha_5-\tfrac{328}{5}\beta_5+\tfrac{16}{3}\alpha_6+\tfrac{32}{3}\beta_6+56\alpha_7\\&+56\beta_7+32\alpha_8-16\beta_8+\tfrac{226}{3}\alpha_9-\tfrac{136}{3}\beta_9\\&+\tfrac{256}{5}\alpha_{10}+\tfrac{144}{5}\beta_{10}) ,\end{aligned} \tag{11}$$

$$\begin{aligned}C_{12}=\frac{1}{a}(&\alpha_1-5\beta_1-4\beta_2+6\alpha_3-30\beta_3+4\alpha_4-20\beta_4\\&+\tfrac{54}{5}\alpha_5+22\beta_5+\tfrac{16}{3}\alpha_6-\tfrac{64}{3}\beta_6-\tfrac{268}{7}\alpha_7+\tfrac{124}{7}\beta_7\\&-16\beta_8+\tfrac{49}{3}\alpha_9-\tfrac{139}{3}\beta_9-80\beta_{10}-8A) ,\end{aligned} \tag{12}$$

TABLE I. Calculated values of radial (α_i) and tangential (β_i) force constants (dyn/cm) for pure metals ($a = 3.5165$ Å for Ni and $a = 3.8829$ Å for Pd).

Set of nearest neighbors	Radial force constants			Tangential force constants		
	Parameter	Ni	Pd	Parameter	Ni	Pd
1	α_1	42 076.75	46 123.42	β_1	−3 503.39	−5 817.9
2	α_2	292.92	1 482.88	β_2	−28.15	21.7
3	α_3	60.23	−504.33	β_3	95.25	99.2
4	α_4	−652.32	−518.00	β_4	10.82	−14.6
5	α_5	182.69	419.81	β_5	−14.28	−10.6
6	α_6	160.37	51.36	β_6	8.27	17.9
7	α_7	−167.57	−319.39	β_7	6.00	2.9
8	α_8	−91.96	−28.70	β_8	−4.64	−10.4
9	α_9	97.87	220.61	β_9	−3.75	−2.9
10	α_{10}	83.72	74.28	β_{10}	2.03	6.0

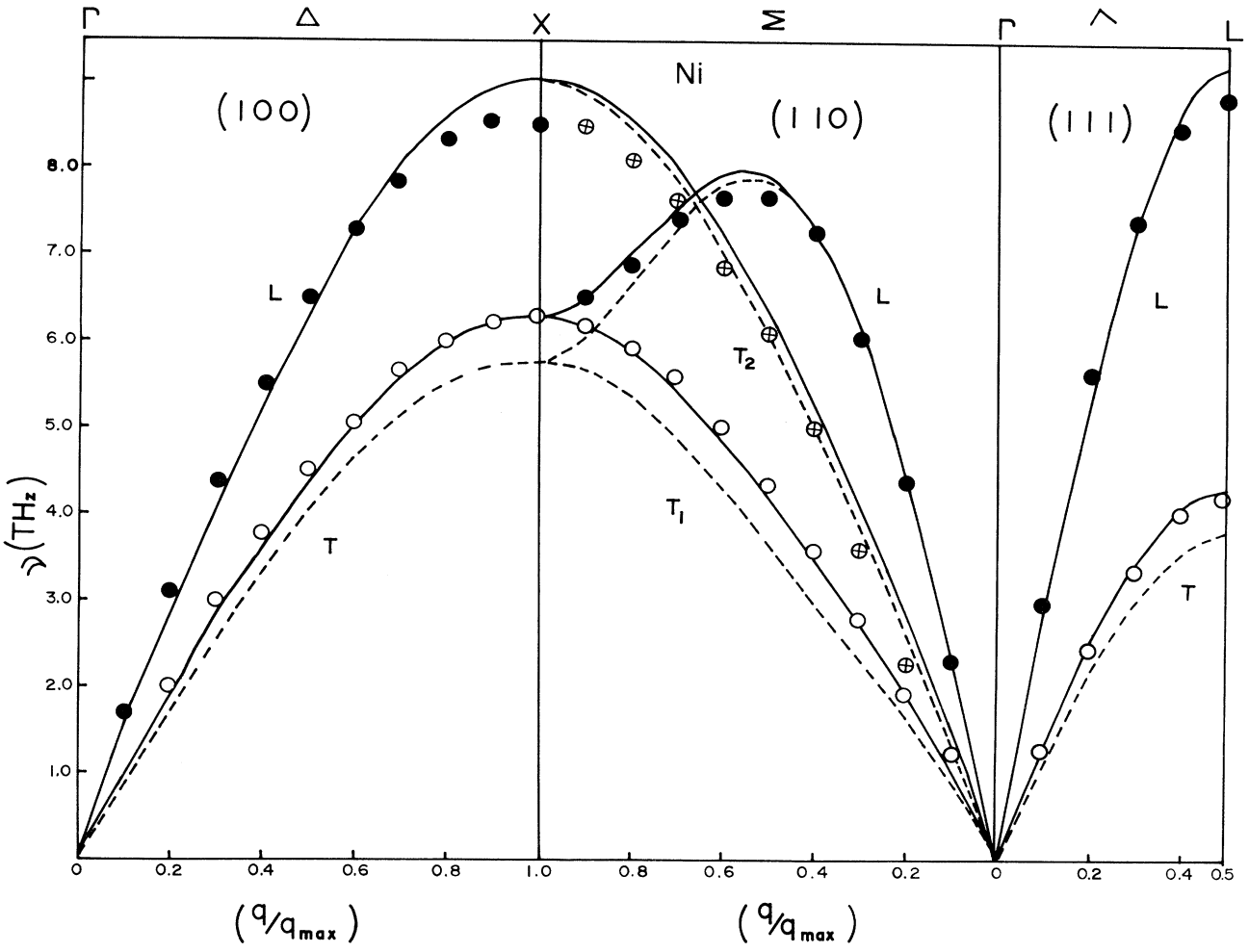

FIG. 1. Phonon dispersion in Ni: dotted curves represent the calculations in second-order pseudopotential theory and solid curves by including three-body forces; ○, ●, ⊕, experimental points of Birgeneau *et al.* (Ref. 1).

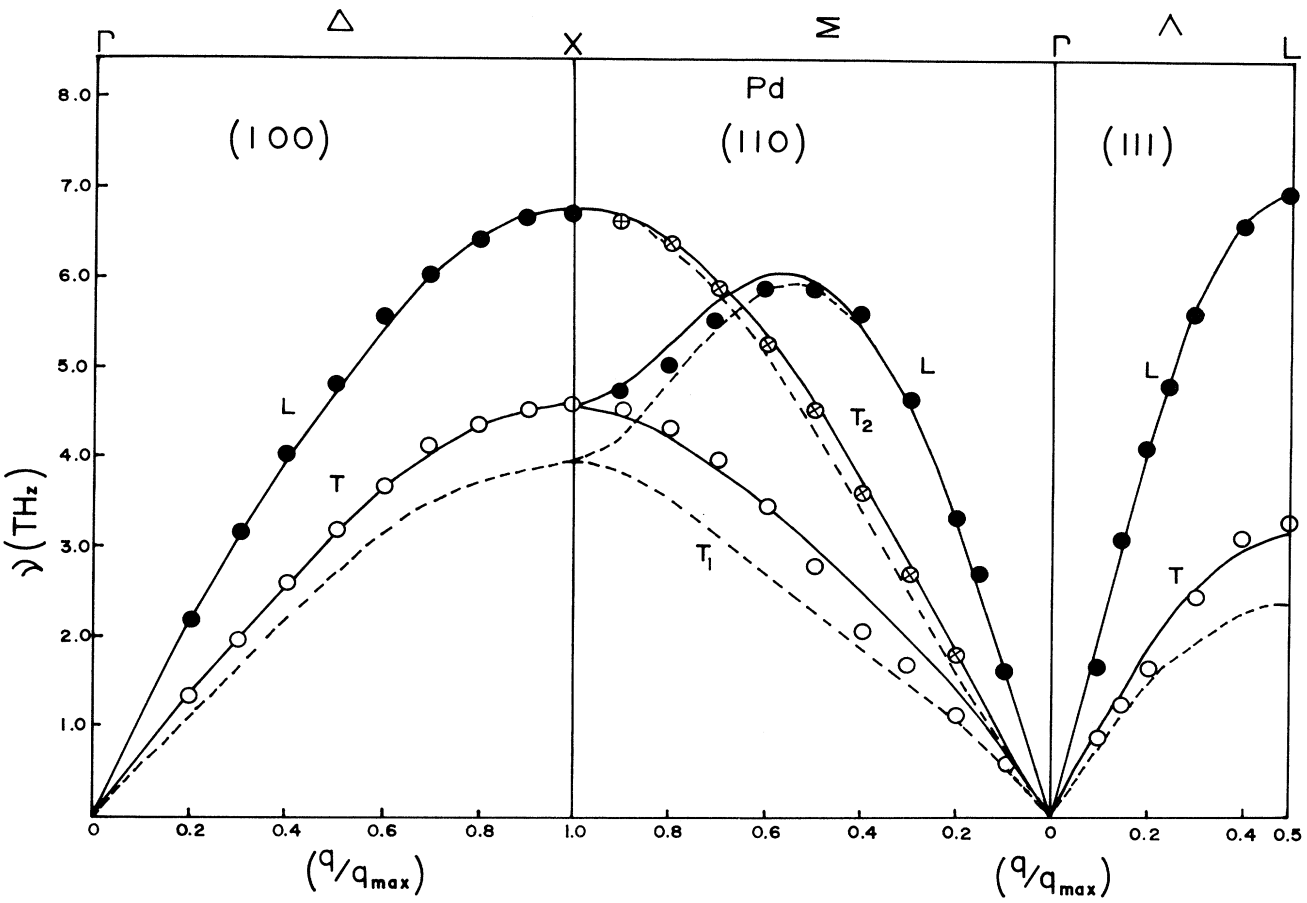

FIG. 2. Phonon dispersion in Pd: dotted curves represent the calculations in second-order pseudopotential theory and solid curves by including three-body forces; ○, ●, ⊕, experimental points of Miller and Brockhouse (Ref. 2).

$$C_{44}=\frac{1}{a}(\alpha_1+3\beta_1+4\beta_2+6\alpha_3+18\beta_3+4\alpha_4+12\beta_4 + \tfrac{18}{5}\alpha_5-\tfrac{182}{3}\beta_5+\tfrac{16}{3}\alpha_6+\tfrac{32}{3}\beta_6+28\alpha_7 + 84\beta_7+16\beta_8+\tfrac{49}{3}\alpha_9+\tfrac{41}{3}\beta_9+\tfrac{64}{5}\alpha_{10} + \tfrac{336}{5}\beta_{10}+4A)\ . \quad (13)$$

These relations are used to compute the elastic constants of pure Ni and Pd as well as those of $Ni_{0.55}Pd_{0.45}$ alloys.

III. NUMERICAL RESULTS AND DISCUSSIONS

First of all we use Eqs. (4)–(6) to calculate the radial and tangential force constants of fcc Ni and Pd by using the TMMP of Animalu[5] in conjunction with the dielectric function due to Hubbard and Sham. This calculation involves second-order terms in electron-ion pseudopotential and, hence, results in the central pairwise forces in the interaction system. These force constants are evaluated at the experimental lattice constants $a=3.5165$ and

TABLE II. Elastic constants of Ni, Pd, and $Ni_{0.55}Pd_{0.45}$ in units of 10^{11} dyn/cm^2.

Elastic constant	Ni			Pd			$Ni_{0.55}Pd_{0.45}$	
	Calculated in second order	Calculated by including three-body forces	Experimental value (Ref. 12)	Calculated in second order	Calculated by including three-body forces	Experimental value (Ref. 13)	Calculated in second order	Calculated by including three-body forces
C_{11}	22.78	22.78	24.60	24.37	24.37	22.70	22.45	22.45
C_{12}	17.84	14.69	15.00	22.47	17.57	17.59	19.43	15.47
C_{44}	8.70	10.28	12.20	6.10	8.55	7.17	7.48	9.46

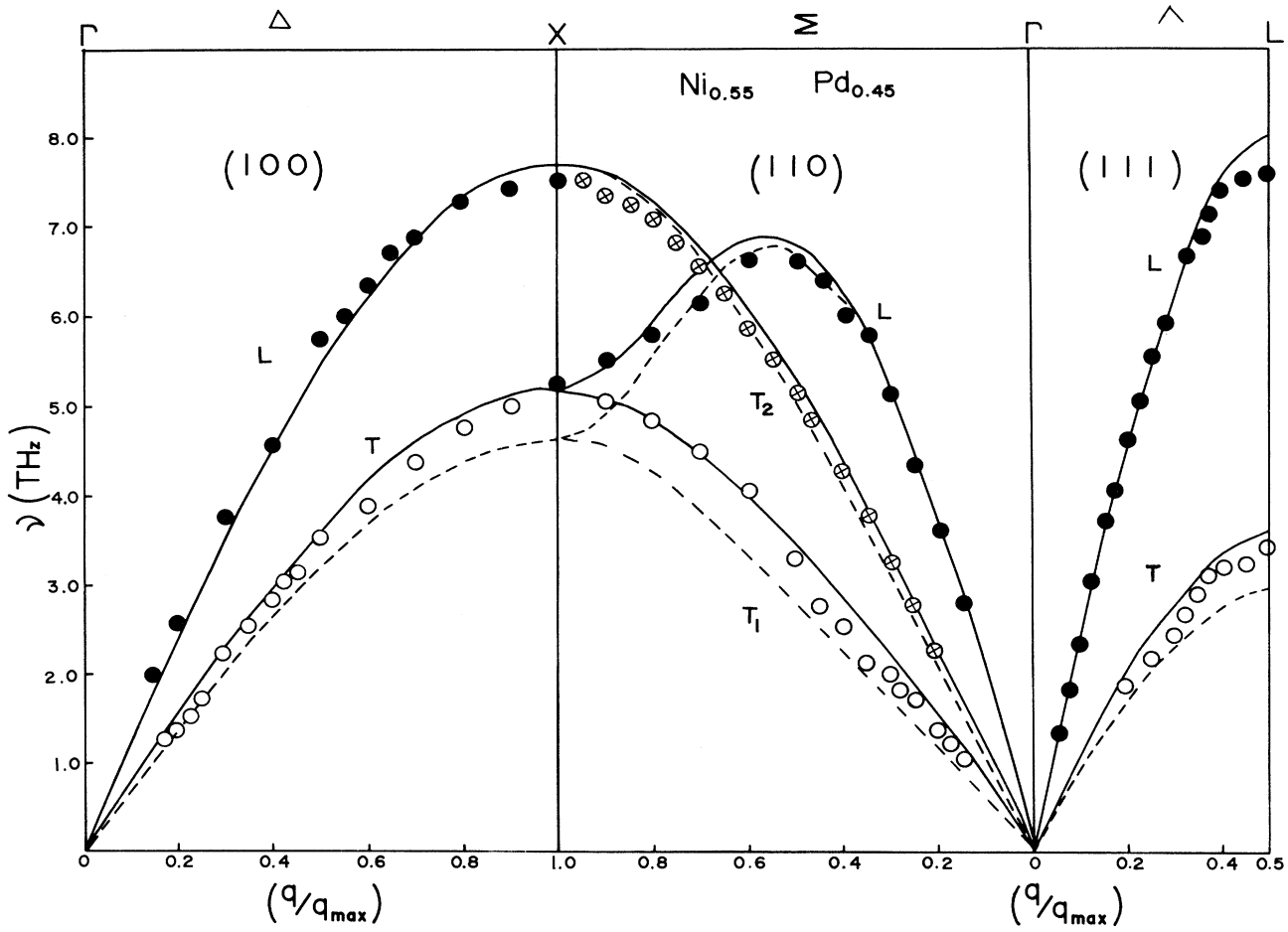

FIG. 3. Phonon dispersion in $Ni_{0.55}Pd_{0.45}$: dotted curves represent the calculations by taking the concentration average of the force consonants of component metals evaluated at the lattice constant of the alloy in the second-order pseudopotential theory and solid curves by including three-body forces; ○, ●, ⊕, experimental points of Kamitakahara and Brockhouse (Ref. 3).

3.8829 Å (Ref. 10) of the pure Ni and Pd crystals, respectively up to 10 sets of nearest neighbors and are presented in Table I. The values of the force constants are then fed into the dynamical matrix and the secular equation (1) is solved to compute the dispersion relations along the three high-symmetry directions [100], [110], and [111]. The phonon dispersion curves, so computed, are plotted in Figs. 1 and 2 for Ni and Pd and compared with the experimental data of Birgeneau *et al.*[1] and Miller and Brockhouse,[2] respectively. The present results for fcc Ni and Pd, using the real-space analysis, are in agreement with those of Animalu[5] using reciprocal analysis. The

TABLE III. Force constants (dyn/cm) for the $Ni_{0.55}Pd_{0.45}$ alloy ($a = 3.6813$ Å).

	Radial force constants				Tangential force constants		
Parameter	Ni	Pd	$Ni_{0.55}Pd_{0.45}$	Parameter	Ni	Pd	$Ni_{0.55}Pd_{0.45}$
α_1	30 994.00	59 862.30	43 984.76	β_1	−2 886.10	−7 928.2	−5 155.08
α_2	1 209.50	1 573.20	1 373.41	β_2	−49.74	44.36	−7.40
α_3	−360.77	−122.60	−253.60	β_3	74.24	136.64	−102.32
α_4	−305.75	−985.05	−611.44	β_4	−8.71	22.71	5.43
α_5	247.06	105.68	183.44	β_5	−1.50	−32.13	−15.29
α_6	−58.31	469.54	179.22	β_6	9.25	6.42	8.87
α_7	−137.25	−135.39	−136.41	β_7	−1.76	19.10	7.63
α_8	57.71	−348.25	−124.07	β_8	−4.38	−1.73	−3.18
α_9	87.04	8.81	51.84	β_9	1.23	−12.14	−4.79
α_{10}	−27.93	255.83	99.67	β_{10}	2.80	−3.41	0.01

maximum errors occur at the zone boundaries for the transverse branches and are 8.7 and 14.1 % along the [100] direction and 9.4 and 26.9 % along the [111] direction for Ni and Pd, respectively.

Next, Eqs. (11)–(13) are used to compute the elastic constants of Ni and Pd and are presented in Table II with the experimental data of Alers *et al.*[11] and Rayne *et al.*[12] The elastic constants C_{11} for the two metals are of the same order of magnitude as the experimental ones, but C_{12} and C_{44} differ from the measured values with a maximum error of 28.7% for C_{44} of Ni metal.

For the computation of the dispersion relations and elastic constants of the fcc $Ni_{0.55}Pd_{0.45}$ alloy before taking the concentration average of the parameters it seems appropriate that the force constants of the component metals Ni and Pd are to be evaluated at the lattice constant of the alloy. The lattice constant of the alloy $Ni_{0.55}Pd_{0.45}$ is calculated using the relation (7) and is obtained to be 3.6813 Å, which is very close to the experimental value 3.72 Å.[3] In the present analysis, therefore, we again use Eqs. (4)–(6) and calculate the force constants of fcc Ni and Pd at $a = 3.6813$ Å for the alloy. These force constants are presented in Table III. Next, Eqs. (8) and (9) are used to determine the force constants of the $Ni_{0.55}Pd_{0.45}$ alloy and the values, so calculated, are given in Table III. The alloy force constants are then fed into the dynamical matrix and the secular equation (1) is solved to calculate the phonon dispersion curves along [100], [110], [111] symmetry directions for the $Ni_{0.55}Pd_{0.45}$ alloy. The computed dispersion relations are presented in Fig. 3 with the experimental data of Kamitakahara and Brockhouse.[3] We find that the phonon dispersion curves are seen in reasonably good agreement with the neutron data with a maximum error of 12 and 14.7 % for the transverse branches of [100] and [111] directions, respectively. The elastic constants C_{11}, C_{12}, and C_{44} are also calculated for the $Ni_{0.55}Pd_{0.45}$ alloy by making use of Eqs. (11)–(13) and are presented in Table II.

An observation at the computed results for the phonon dispersion of Ni, Pd, and $Ni_{0.55}Pd_{0.45}$ shows that the maximum errors at the zone boundary of the [100] direction are 8.7, 14.1, and 12.0 % and those of the [111] directions are 9.4, 26.9, and 14.7 %, respectively. Therefore, the mean-crystal model works approximately well for the high-concentration alloy $Ni_{0.55}Pd_{0.45}$. As far as

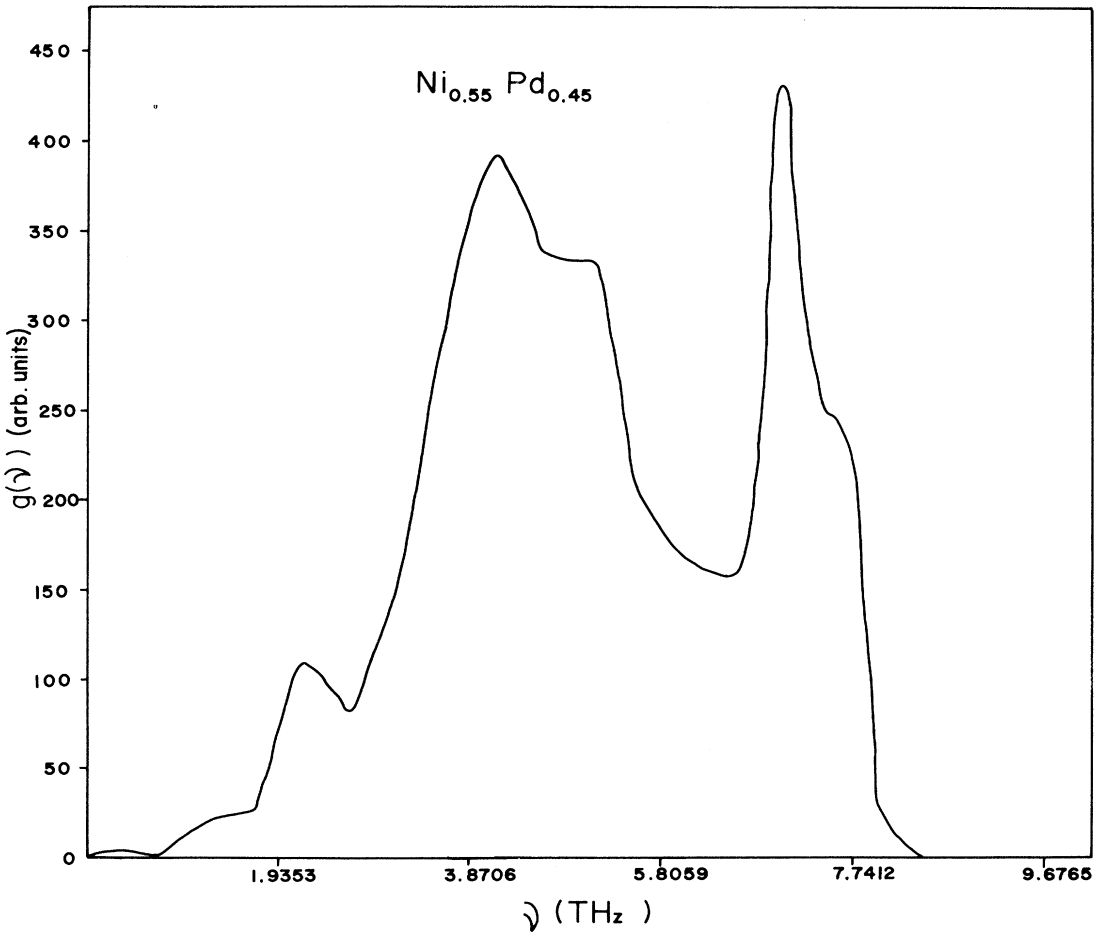

FIG. 4. Phonon density of states of the $Ni_{0.55}Pd_{0.45}$ alloy.

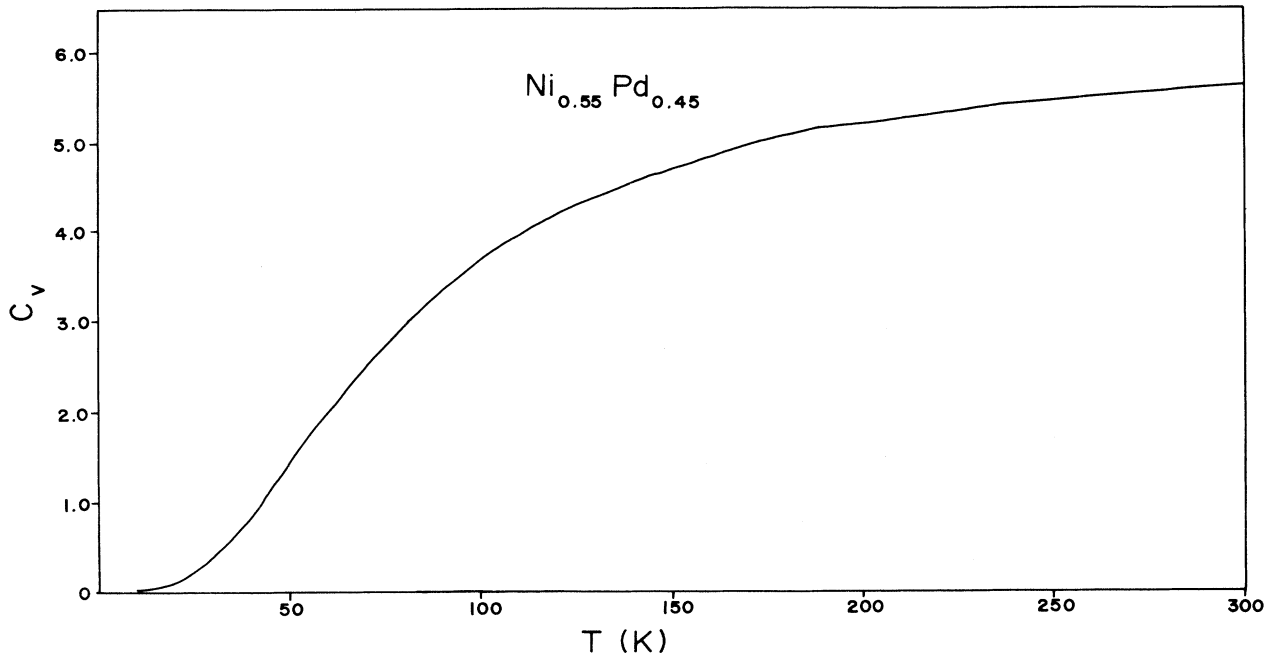

FIG. 5. Variation of specific heat of the $Ni_{0.55}Pd_{0.45}$ alloy with temperature.

the elastic constants are concerned, the computed elastic constants C_{11} for the three metallic systems are of the same order of magnitude and the calculated values of C_{12} and C_{44} for the $Ni_{0.55}Pd_{0.45}$ alloy are approximately satisfying the concentration average of the elastic constants of the component metals.

Next, we incorporate the effect of three-body forces in the dynamical matrix and elastic constant relations. In view of the work of Upadhyaya and Prakash,[6] we obtain the value of the three-body force constant by fitting to the zone-boundary phonon frequency of the [100] direction of the transverse branch. This involves one parameter A

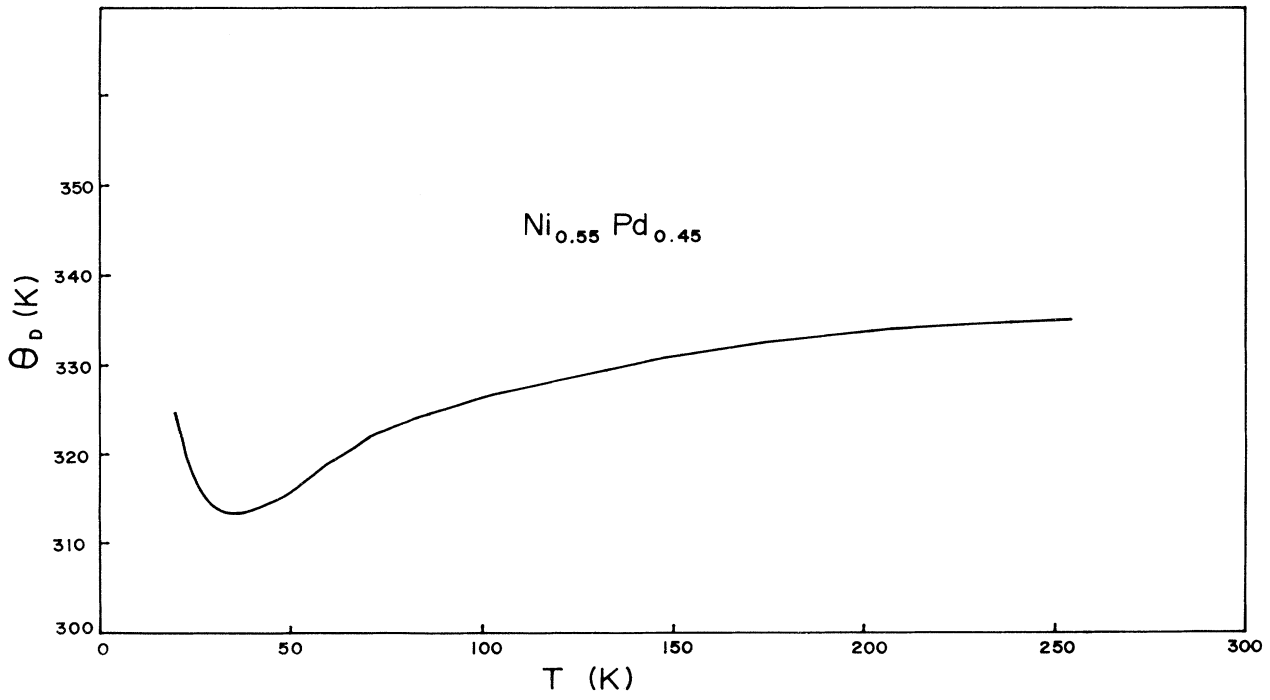

FIG. 6. Temperature dependence of the Debye temperature for the $Ni_{0.55}Pd_{0.45}$ alloy.

and its value is found to be 1385.8 and 2378.0 dyn/cm for Ni and Pd, respectively. For the $Ni_{0.55}Pd_{0.45}$ alloy, the three-body force constant was not fitted to the phonon frequency but was obtained by the linear relation with the value $A = 1823.3$ dyn/cm. Now, by including for the three-body effects in the dynamical matrix, the secular equation is again solved along the [100], [110], and [111] symmetry directions for Ni, Pd, and $Ni_{0.55}Pd_{0.45}$ metallic systems and the phonon dispersion curves are plotted along the three directions for the three cases. The results of computation are presented in Figs. 1–3 by solid curves for Ni, Pd, and $Ni_{0.55}Pd_{0.45}$, respectively. We find that in all the three cases, an almost exact agreement is obtained with the experimental data. The calculations were also done for elastic constants by including three-body forces. The present form of the three-body potential does not affect the elastic constant C_{11}, but, in general, the C_{12} and C_{44} elastic constants for the metallic systems are changed in the right direction to give a close agreement with the experimental values (Table II).

The phonon density of states for the $Ni_{0.55}Pd_{0.45}$ alloy is computed by incorporating three-body forces in the system in the root sampling method as discussed in Ref. 13 and the results of computation are presented in Fig. 4. We find that the phonon density of states has similar trends to that of Kamitakahara and Brockhouse.[3] Further, we have also computed the specific heat and Debye temperature as a function of temperature from the density of states by following the standard procedure and presented the results of computation in Figs. 5 and 6.

Recently, Garg *et al.*[14,15] have adopted a similar procedure for the calculation of the lattice dynamics of fcc disordered binary alloys. They use de Launay's angular force model[16] for the calculation of force constants of component metals, assuming the interatomic forces effective up to second-nearest neighbors and then they take the concentration average of the force constants and masses of the end members to study the dynamical behavior of disordered alloy. Thus, these workers essentially use short-range forces to study the lattice dynamics of metallic systems. However, the interatomic forces in metallic systems are known to possess long-range character. Further, it is to be pointed out that the force constants of the component metals in these works are evaluated by fitting with the experimental data for phonon frequencies and elastic constants. In the present work, on one hand, we determine the *ab initio* radial and tangential force constants by using the TMMP of Animalu[5] and, on the other, we reasonably account the long-range character of interatomic forces by considering the interaction system extending up to 10 sets of nearest neighbors. Further, as far as the central pairwise forces are concerned, no parameter is fitted with any lattice dynamical or elastic property. In this respect, the present analysis is also relatively much more satisfactory than those of Kamitakahara and Brockhouse[3] and Upadhyaya and Shyam.[4]

Thus, in the present work, we evaluate the *ab initio* radial and tangential force constants of two fcc transition metals Ni and Pd by using the transition-metal model potential of Animalu.[5] A real-space analysis is done for the calculation of phonon dispersion and elastic constants of the two metals by considering the interatomic forces effective up to 10 sets of nearest neighbors. In order to study the phonon and elastic properties of $Ni_{0.55}Pd_{0.45}$ alloy, the force constants of fcc Ni and Pd are again evaluated at the lattice constant of the alloy and the concentration averages of these force constants and masses of the constituent metals are used to compute the dispersion relations and elastic constants. For the three metallic systems, Ni, Pd, and $Ni_{0.55}Pd_{0.45}$, the longitudinal branches of the phonon dispersion curves are relatively in closer agreement than the transverse branches. When three-body forces are incorporated in the metallic systems, close agreement is also found between the experimental and computed transverse branches but at the cost of one disposable parameter.

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