Microscopic Theory of Dielectric Screening and Lattice Dynamics in the Wannier Representation. II. Model Application to the Transition Metals Pd and Ni [†]

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The unified theory of lattice dynamics in the Wannier representation, presented in a previous paper, is here used to calculate the phonon dispersion of the transition metals Pd and paramagnetic Ni. This application represents the first microscopic phonon calculation in transition metals which takes into account the local field effects in the d-electron response. Using a tight-binding model for the d electrons and a nearly-free-electron description for the s electrons it is shown that these effects give contributions to the longitudinal-phonon branches and to the elastic constants C_{11} and C_{12} of the same order of magnitude as the Hubbard-exchange corrections (10–20%).

I. INTRODUCTION

Transition metals present, as an intermediate case between simple metals and insulating crystals, an interesting and appealing possibility for testing the unified approach to lattice dynamics, developed in the preceding paper[1] (hereafter referred to as I). The main reason for this stems from the fact that the conduction electrons of these metals are of free-electron (s- and p-like) character as well as of localized (d-like) character. Moreover, the d-like electrons of the filled bands are not rigidly bound to the core and therefore must be included in a calculation of the dielectric response. As a result, the dielectric matrix ϵ contains a free-electron contribution $\epsilon_0(\vec{q}+\vec{G})$, which is diagonal in the reciprocal lattice vectors $\vec{G}$ and $\vec{G}'$, and also a nondiagonal ($\vec{G} \neq \vec{G}'$) part, which is due to the d-type electronic states. The nondiagonal contribution leads to the ($\vec{G} \neq \vec{G}'$) terms in the dynamical matrix of Paper I and corresponds to local-field or crystal structure effects in the dielectric response.

The first microscopic phonon calculation which properly took into account this mixed nature of the electronic states in combination with the resulting nondiagonality of the dielectric matrix was performed on the transition metal Ni in the paramagnetic phase.[2] In this paper we shall discuss the relationship between the results of our former treatment of Ni (which was only briefly sketched in Ref. 2) and those of our present calculation of Pd where we investigate as well the influence of exchange effects on the phonon spectrum. The model of the band structure which we introduce for Pd is similar in its general features to the model employed in the case of Ni. The electronic energies are assumed to be given in the effective mass approximation while for the corresponding wave functions a tight-binding scheme is applied to the $4d$ electrons and the free-electron approximation is used for the electrons in the $5s$ band. It is found that the contributions to ϵ which are due to inter-

band transitions are of the order of $\frac{1}{10}$ smaller than the intraband contributions of the unfilled s and d conduction bands. Therefore we neglect all interband transitions in the dielectric matrix and use a noninteracting s-d two-band model for the band structure. We shall see that too much emphasis has been given in the basic formulation to the core electrons which rigidly move with the nuclei. This can be remedied by the use of an effective electron-ion potential which we approximate by a local pseudopotential. We give a careful treatment of the screening of this effective potential by s as well as d electrons,[3] in contrast to previous work where the d-electronic screening is neglected,[4] or treated in an inappropriate approximation.[5] We then derive the dynamical matrix in terms of the inverse dielectric matrix and calculate the phonon frequencies of the paramagnetic transition metal Pd. The remainder of the paper is devoted to presenting the results of this phonon calculation and discussing them with our previous Ni results.

Because of the simplicity of the band-structure model and the local pseudopotential, we do not claim to calculate quantitatively the absolute magnitude of the phonon frequencies in Pd and Ni. The present calculations provide a first step in applying the formalism of Paper I. But the important point to be emphasized is that we clearly show how local-field corrections due to the d electrons, i.e., nondiagonal elements of the dielectric matrix, enter in an explicit calculation and that they are essential for a satisfactory explanation of the phonon dispersion of the transition metals Pd and paramagnetic Ni.

II. MODEL BAND STRUCTURE AND DIELECTRIC MATRIX

We begin by constructing a band model for the transition metal Pd which is related in its general features to the model introduced by Prakash and Joshi in their calculation of the diagonal dielectric function of Ni.[6] Our model is based on recent aug-

mented-plane-wave results of Mueller *et al.*[7] but it does not explicitly take into account the s-d hybridization which splits s and d bands. Thus the s bands are constructed by joining the energy point Γ_1 to X'_4, Γ_1 to K_1, and Γ_1 to L'_2 in the symmetry directions Δ, Σ, and Λ, respectively. For d bands, Γ_{12} is joined to X_1 in the Δ direction, Γ_{12} and Γ'_{25} are joined with upper and lower K_1, respectively, in the Σ direction, and Γ'_{25} is joined with L_1 in the Λ direction (see Fig. 1). The noninteracting bands obtained in this manner are then approximated by parabolic bands centered at the Γ point. The effective masses for the s and d subbands which intersect the Fermi level E_F are calculated by means of the relations

$$m_s = \frac{\hbar^2 k_{F,s}^2}{2[E_F - E(\Gamma_1)]}, \quad m_d = \frac{\hbar^2 k_{F,d}^2}{2[E_F - E(\Gamma'_{25})]} \quad (1)$$

with $k_{F,s} = (3\pi^2 Z_s/\Omega_0)^{1/3}$ and $k_{F,d} = (3\pi^2 Z_d/\Omega_0)^{1/3}$, where $k_{F,s}$ and $k_{F,d}$ are the Fermi radii of the subbands. The numbers of s and d electrons per unit cell of volume Ω_0, Z_s and $Z_d = 2 - Z_s$, are taken as 0.4 and 1.6, respectively, in agreement with the de Haas–van Alphen studies of Vuillemin[8] and the augmented-plane-wave (APW) results of Mueller *et al.* The calculation of the average effective masses for filled d subbands and the assignment of these subbands with different magnetic quantum numbers both proceed along the lines given in Ref. 6.

The Bloch functions corresponding to our simplified band description are approximated by plane waves in the $5s$ band
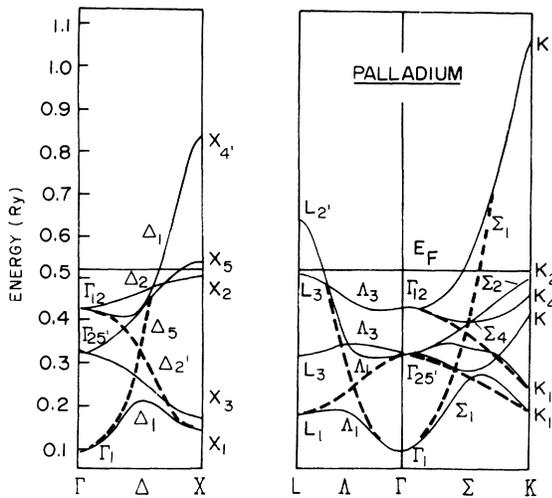

FIG. 1. Model of the noninteracting band structure for Pd. The solid lines give the results of the APW calculation of Mueller *et al.*, while the dashed lines describe the noninteracting bands.

$$\psi_{s,\vec{k}}(\vec{r}) = \frac{1}{(N\Omega_0)^{1/2}} e^{i\vec{k}\cdot\vec{r}}, \quad (2)$$

while a tight-binding ansatz of the form

$$\psi_{d,m\vec{k}}(\vec{r}) = \frac{1}{N^{1/2}} \sum_l e^{i\vec{k}\cdot\vec{R}^l} \varphi_{dm}(\vec{r} - \vec{R}^l) \quad (3)$$

is used for the $4d$ wave functions, where the sum runs over all lattice vectors $\vec{R}^l$. We take the atomic orbitals $\varphi_{dm}(\vec{r})$ for the neutral Pd atom from the Hartree-Fock calculations of Gómbas and Szóndy.[9] Integrating the square of these orbitals over the unit cell yields a value of about 0.95, where the atomic orbitals are normalized over all space. Thus the overlap matrix elements $A_s(\vec{q}+\vec{G})$ of Eq. (12) in Paper I may be expected to decrease rapidly with increasing lattice vectors $\vec{R}^l$. Consequently we take into account only the interactions of orbitals situated on the same atom in evaluating the dielectric matrix, Eq. (12) of I.

The model for the electronic structure of Pd we have now constructed involves two types of transitions for a readjustment of electrons in an external field: (a) intraband transitions in the unfilled s and d bands, and (b) interband transitions from filled d subbands to s and d conduction bands, and interband transitions between s and d conduction bands. The calculation of the s-s intraband contribution to the dielectric matrix is straightforward and gives the well-known Lindhard formula ($T = 0\,°$K)

$$\epsilon_0(\vec{q}+\vec{G}) = \delta_{\vec{G},\vec{G}'} - v(\vec{q}+\vec{G})\frac{N\Omega_0 m_s k_{F,s}}{2\pi^2\hbar^2}$$

$$\times\left(1 + \frac{4k_{F,s}^2 - |\vec{q}+\vec{G}|^2}{4k_{F,s}|\vec{q}+\vec{G}|}\ln\left|\frac{2k_{F,s}+|\vec{q}+\vec{G}|}{2k_{F,s}-|\vec{q}+\vec{G}|}\right|\right).$$

$$(4)$$

This result shows the simplicity of the free-electron treatment of simple metals, as the matrix ϵ collapses into the scalar dielectric function ϵ_0 for a free-electron gas. But in our model off-diagonal contributions to the dielectric matrix corresponding to "local-field corrections" arise because of the presence of tight-binding d electrons. The contribution of the $4d$ intraband scattering processes may be calculated by using Eqs. (12) of I and (3) leading to the expression[10]

$$\epsilon_{d,d}(\vec{q}+\vec{G}, \vec{q}+\vec{G}') = -v(\vec{q}+\vec{G})A(\vec{q}+\vec{G})N(\vec{q})A^*(\vec{q}+\vec{G}'),$$

where

$$A(\vec{q}+\vec{G}) = \int_{N\Omega_0} \varphi_{dm}^*(\vec{r}) e^{-i(\vec{q}+\vec{G})\vec{r}} \varphi_{dm}(\vec{r}) d^3r \quad (5)$$

and

$$N(\vec{q}) = \sum \frac{f(dm, \vec{k}) - f(dm, \vec{k}+\vec{q})}{E(dm, \vec{k}) - E(dm, \vec{k}+\vec{q})} = -\frac{m_{dm}k_{F,d}N\Omega_0}{2\pi^2\hbar^2}$$

$$\times\left(1 + \frac{4k_{F,d}^2 - q^2}{4k_{F,d}\cdot q}\ln\left|\frac{2k_{F,d}+q}{2k_{F,d}-q}\right|\right).$$

If we assign to the $4d$ conduction band the magnetic quantum number $m = 1$, then the overlap matrix element $A(\vec{q} + \vec{G})$ is given by the relation

$$A(\vec{q} + \vec{G}) = X_0 - \tfrac{2}{7}(5\pi)^{1/2} Y_0^{2*}(\theta, \varphi) X_2$$
$$- \tfrac{8}{7}(\pi)^{1/2} Y_0^{4*}(\theta, \varphi) X_4 . \tag{6}$$

In this formula $Y_m^l(\theta, \varphi)$ denotes the spherical harmonic with quantum numbers l and m. The integrals X_l defined by

$$X_l = \int_0^\infty j_l(|\vec{q} + \vec{G}| r) R_{4d}^2(r) \, dr , \tag{7}$$

where $j_l(|\vec{q} + \vec{G}| r)$ is the spherical Bessel function of order l, may be solved analytically[11] by using the Gómbas radial function for the $4d$ states of Pd

$$R_{4d}(r) = -301.4 r^3 e^{-9.285r} + 26.23 r^{2.5} e^{-3.251r} . \tag{8}$$

The final expressions are very lengthy, but are otherwise easy to calculate and we shall not write them down.

In a similar way the remaining interband contributions to the dielectric matrix, $\epsilon_{d,s} + \epsilon_{s,d}$, may be calculated. We found that in the symmetry directions Δ, Σ, and Λ the magnitude of these contributions is small (with a maximum value of about 10% at the Brillouin zone faces) in comparison to the magnitude of the intraband contributions, $\epsilon_0 + \epsilon_{d,d}$. We therefore neglect $\epsilon_{d,s}$ and $\epsilon_{s,d}$ in our explicit phonon calculation and retain only the conduction-band contributions given by Eqs. (4) and (5).[12]

In this effective s-d two-band model the inverse dielectric matrix is given by [see formula (13) of Paper I]

$$\epsilon^{-1}(\vec{q} + \vec{G}, \vec{q} + \vec{G}') = \frac{1}{\epsilon_0(\vec{q} + \vec{G}')} \left(\delta_{\vec{G}, \vec{G}'} + \frac{v(\vec{q} + \vec{G})}{\epsilon_0(\vec{q} + \vec{G})} \right.$$

$$\left. \times \frac{A(\vec{q} + \vec{G}) A^*(\vec{q} + \vec{G}')}{N^{-1}(\vec{q}) - \sum_{\vec{H}} |A(\vec{q} + \vec{H})|^2 v(\vec{q} + \vec{H})/\epsilon_0(\vec{q} + \vec{H})} \right) \tag{9}$$

Because of the choice of the polar axis and the use of spherical harmonics, the dielectric matrix constructed does not exhibit the symmetry of the crystal. To satisfy these symmetry requirements we calculate the matrix element $A(\vec{q} + \vec{G})$ by averaging with equal weighting over all five quantum numbers m. This leads to the substitution $A(\vec{q} + \vec{G}) = X_0$ in Eq. (6). An average of this form has independently been introduced by Brown[4] in his calculation of the dielectric matrix of Pd using a similar s-d two-band model. In the Prakash and Joshi calculation of the phonon dispersion in paramagnetic Ni,[5] in which only diagonal s- and d-electron screening was taken into account (we shall discuss this paper in more detail subsequently), the approximation $A(q, \theta, \varphi) = A(q, 0, 0)$ compensates for the erroneous choice $m = 1$ for the magnetic quantum number of the d band.

III. LATTICE DYNAMICS

We have now assumed a rigid-ion core of configuration $(4d)^8$ which does not deform in the perturbing phonon field, whereas in Paper I the dynamical matrix was derived treating all electrons equivalently. From the excitation spectrum of the crystal it is clear that only a certain part of the electrons can be responsible for the "dynamical" interatomic forces while all the remaining electrons do move bodily with the nuclei. This splitting becomes apparent in our dielectric formalism from the fact that the contribution of the dynamical electrons, or valence electrons, to the dielectric matrix ϵ is large compared to the remaining contributions.

A theory which emphasizes the special role of the valence electrons is the pseudopotential theory. Here one neglects completely the distortion of the core-electron wave functions arising from the nuclear displacements and the effect on the valence electrons which results from this distortion. But one takes into account the Pauli principle in that the wave functions of the dynamical electrons must be orthogonal to the core-electron wave functions. The effect of the orthogonalization in the core region is simulated by a repulsive potential which largely cancels the attractive core potential. In general this repulsive potential is of nonlocal character[13] and thus leads to a very complicated expression for the dynamical matrix.[14] In our explicit phonon calculation we replace the nonlocal pseudopotential by a parametrized local model potential. This is a good approximation for the free-electron-like s states. However, for the d-type states of our band scheme, the repulsive part vanishes because the tight-binding wave functions are already orthogonal to the core wave functions. Consequently, the potential seen by the d-like electrons should be replaced within the framework of the s-d two-band model by the bare ionic potential $(4\pi Z e^2 / N\Omega_0 q^2)$. Taking into account this difference between s- and d-repulsive potentials in our actual phonon calculation introduces no significant deviation (less than 5%) from the results presented in Figs. 2 and 3. Therefore, and also in view of the parametrized character of the pseudopotential, we do not think it worthwhile to keep the different behavior of the s and d pseudopotentials in our following work. Within this local pseudopotential approach the electronic contribution to the phonon self-energy may be calculated by means of a Goldstone expansion including electron-phonon interactions.[15] Neglecting core-core overlap and approximating the corresponding interaction potential by a simple Coulomb potential with effective charge $Z = 2$ (see above for comments on the number of s and d electrons per s and d conduction bands) results finally in the following expression for the

Lattice parameter	a_0	7.3515	Effective mass	m_s	0.5731
Volume of unit cell	Ω_0	99.3272	Effective mass	m_d	3.2053
Mass of an atom	M	19.385×10^4	Strength of pseudopotential	β	23.4
Fermi radius	$k_{F,s}$	0.4920	Decay radius	ρ	0.1
Fermi radius	$k_{F,d}$	0.7812			

dynamical matrix

$$\overline{D}_{\alpha\beta}(\vec{q}) = \frac{4\pi Z^2 e^2}{\Omega_0} \sum_{\vec{G}} \frac{(\vec{q}+\vec{G})_\alpha (\vec{q}+\vec{G})_\beta}{|\vec{q}+\vec{G}|^2}$$

$$+ N \sum_{\vec{G},\vec{G}'} (\vec{q}+\vec{G})_\alpha V(\vec{q}+\vec{G})$$

$$\times \chi(\vec{q}+\vec{G}, \vec{q}+\vec{G}') V(\vec{q}+\vec{G}')(\vec{q}+\vec{G}')_\beta . \quad (10)$$

We note that this formula is identical in structure to the result given in Eq. (14) of Paper I for the dynamical matrix of an electron-nucleus system. But in Eq. (10) the density response matrix

$$\chi(\vec{q}+\vec{G}, \vec{q}+\vec{G}') = v^{-1}(\vec{q}+\vec{G})[-\delta_{\vec{G},\vec{G}'} + \epsilon^{-1}(\vec{q}+\vec{G}, \vec{q}+\vec{G}')]$$

corresponds only to electron-hole polarizations of s- and d-type electrons which are not included in a formation of the "ions." The inverse dielectric matrix ϵ^{-1} can be taken from Eqs. (4)–(9). Likewise the potential $V(\vec{q})$ in Eq. (10) is the Fourier transform of the local pseudopotential

$$V(\vec{q}) = -\frac{4\pi Z e^2}{N\Omega_0 q^2} + \frac{\beta}{N\Omega_0 (1+\rho^2 q^2)^2} \quad (11)$$

where the first term represents the Coulomb potential due to the ionic charge Ze ($Z = 2$), while the second part describes in a phenomenological way the repulsive part of the potential. In our phonon calculation the parameters β and ρ are adjusted to obtain best agreement with the measured elastic constants C_{11} and C_{44}. The resulting values of β and ρ and the band structure and crystallographical data we used for Pd are in Table I. Results of our phonon calculations in Pd along the symmetry directions $\Delta(100)$, $\Sigma(110)$, and $\Lambda(111)$ are shown in Fig. 2 and compared with the experimental results of Miller and Brockhouse.[16] The solid lines represent a calculation in which exchange effects among the s and d conduction electrons are included in the Hubbard approximation; i.e., the bare electron-electron interaction $v(q) = 4\pi e^2/N\Omega_0 q^2$ in Eqs. (9) and (10) is replaced by

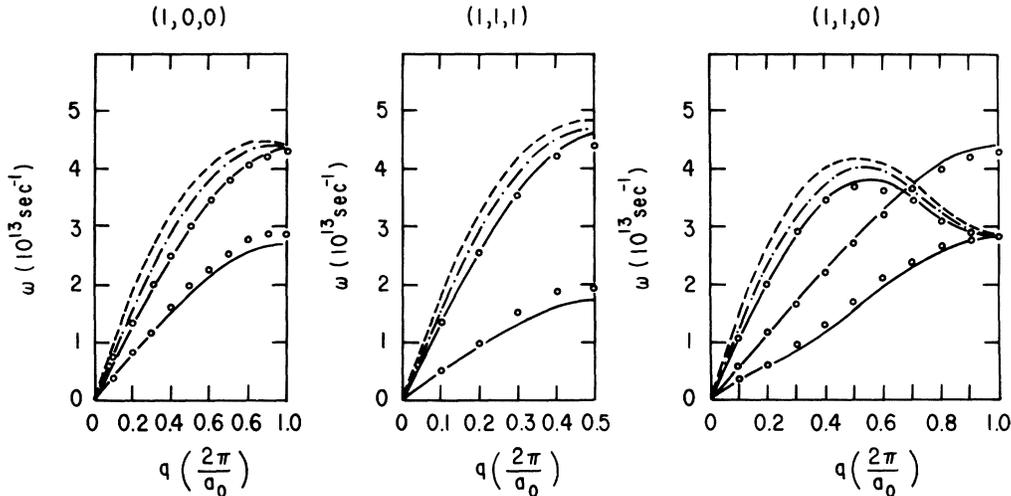$$v(\vec{q})[1 - f(\vec{q})] . \quad (12)$$

FIG. 2. Phonon dispersion curves for Pd (296 °K). Circles denote the experimental phonon frequencies. The solid curves represent the results obtained with the help of the dynamical matrix, Eq. (10), including local-field and Hubbard-exchange corrections. The dash-dotted curves give the results of the same calculation but without exchange correction, and finally the dashed lines represent the free-electron results [$\epsilon = \epsilon_0(\vec{q}+\vec{G})$].

The function $f(\vec{q})$ accounts approximately for the exchange processes between electrons of parallel spin and according to Hubbard[17] is chosen to be

$$q^2/2(q^2 + k_{Fs,d}^2) . \tag{13}$$

For s-electron exchange [i.e., for the electron-electron interaction $v(\vec{q})$ occurring in the scalar function $\epsilon_0(\vec{q})$ and in the corresponding free-electron dynamical matrix] $k_{Fs,d}$ is taken to be $k_{F,s}$, the Fermi radius of the $5s$ band, while for d-electron exchange $k_{Fs,d}$ is replaced by the Fermi radius $k_{F,d}$ of the $4d$ band. In the tight-binding approximation for the d electrons, the most important exchange effect in the d-electronic system is the exclusion of two electrons with the same spin from occupying the same orbital on the same site.[3] Thus, an alternative way of including the d-d exchange is to remove such a contribution from the d-electron screening (this local exchange approximation is equivalent to the $q \to \infty$ limit of the Hubbard correction). Results of a corresponding phonon calculation, which we do not present here, agree to within 5% with the results of the Hubbard treatment shown in Fig. 2. The agreement between these Hubbard results and the measured phonon frequencies is better than 5% with the exception of high q values in the transverse branches of $\Delta(100)$ and $\Lambda(111)$ direction. If the adjusted pseudopotential parameters β and ρ, given in Table I are again used in a new calculation where exchange effects are neglected $[f(\vec{q}) \equiv 0]$, we get the dash-dotted results of Fig. 2. If we finally treat the lattice dynamics of Pd in the free-electron model of simple metals, i.e., take into account only the scalar Lindhard function

$\epsilon_0(\vec{q})$ in Eq. (9), we obtain the dashed lines. Combining these Pd results and comparing them with our former Ni results[2] shown in Fig. 3, we can state the following:

(a) Transverse branches are not renormalized by d-type contributions to the dynamical matrix because in fcc (Ni and Pd) and bcc crystals the diagonal contribution $(\vec{G} = \vec{G}')$ cancels the nondiagonal contribution in the T branches by symmetry. Consequently the renormalization of the transverse branches and of the dielectric constant C_{44} is completely due to the s-type electrons. This fact primarily accounts for the difficulty of the Prakash and Joshi[5] calculation in Ni (given by the dashed lines in Fig. 3) to agree well with experiment, especially in the transverse branches. These authors used a similar s-d two-band model, as we did in Ni and Pd, and also the local pseudopotential approach. But they neglected completely off-diagonal elements of the dielectric matrix, i.e., local-field effects due to the d-electronic response. As a result their T branches are renormalized by diagonal d contributions and are lowered by as much as 20%. In the longitudinal branches diagonal and nondiagonal d-type elements in the dynamical matrix sum up to a maximum of 20%. They are important for the description of the elastic constants C_{11} and C_{12} as well as for the dispersion at q values in the middle of the Brillouin zone.

(b) Taking into account exchange effects in the Hubbard approximation results in a lowering of the longitudinal branches in Pd by about 15%, while the transverse branches are again not influenced by these effects.
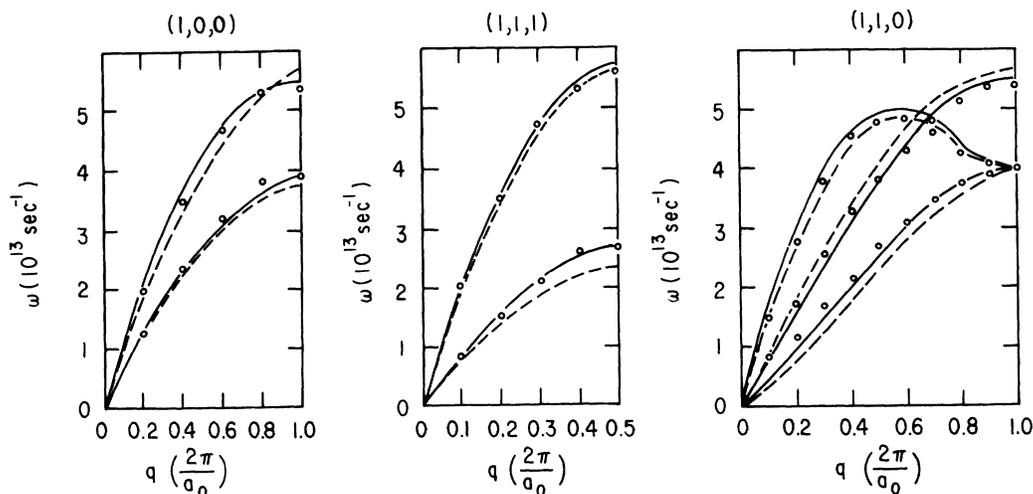

FIG. 3. Phonon dispersion curves for Ni (296 °K). Open circles are the phonon energies measured by Birgeneau *et al.* (Ref. 18). Solid lines give the results of our microscopic phonon calculation, including local-field effects in the electronic screening [$\epsilon = \epsilon(\vec{q} + \vec{G}, \vec{q} + \vec{G}')$]. Dashed lines represent the Prakash and Joshi results [$\epsilon = \epsilon(\vec{q} + \vec{G})\delta_{\vec{G},\vec{G}'}$].

IV. SUMMARY AND DISCUSSION

In the application of the theory developed in Paper I to the transition metals Pd and paramagnetic Ni (the Ni results have already been presented in Ref. 2) we had to introduce a number of approximations in order to reduce the enormous computational work necessary in a phonon calculation with a non-diagonal dielectric matrix.

We started in Sec. II by constructing a noninteracting band model for Pd in which the s-d hybridization which splits the s and d bands was neglected. For the energy dispersion of this simplified band model we assumed an isotropic effective-mass description. From the band-structure calculations this parabolic band model may be seen to be a good approximation for the s-type energy band, but it gives only a rough picture of the non-isotropic behavior of the d-bands. We then calculated within this band-structure model the various contributions to the dielectric matrix and found that the interband contributions are small (less than 10%) compared to the intraband contributions. Therefore our final phonon calculations were based on an s-d two-band model with only intraband transitions retained. For the corresponding wave functions the free-electron approximation was used for the s-type Bloch waves while a tight-binding scheme was applied to the d states. We neglected the mutual orthogonalization of these wave functions which reduces the perfect localization of the d functions, because this delocalization should again be of the order of the interband coupling. But the orthogonalization of the s and d wave functions to

the core states was taken into account within a local pseudopotential approach which gives a qualitatively correct description for the s electrons, whereas for the d-type pseudopotential this local approach is a crude approximation. Exchange effects among s and d conduction electrons were included within the Hubbard approximation commonly used for simple metals.

Results of the corresponding phonon calculations were presented and discussed in Sec. III. The calculated phonon frequencies in Pd and Ni differ from experiment not more than 5% with the exception of the T branches of Δ and Λ direction in Pd. The d-type elements of the dynamical matrix give contributions in the L branches up to 20% and are important for a description of the elastic constants C_{11} and C_{12} as well as for the phonon dispersion in the middle of the Brillouin zone. Unlike the L branches, the T branches and the elastic constant C_{44} are renormalized only by s-electron screening because in these branches the diagonal $(\vec{G} = \vec{G}')$ and nondiagonal d contributions cancel exactly by symmetry. Also the exchange effects in the Hubbard approximation enter only the L branches and here give corrections which are of the same order of magnitude as the d-type contributions.

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is of the separable form as in Eq. (5).

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[12] See also the calculations by Prakash and Joshi for Ni (Ref. 6), where it has been shown that the diagonal s-d contributions to $\epsilon(\vec{q} + \vec{G}, \vec{q} + \vec{G})$ at the Brillouin-zone faces in the symmetry directions give about a 3% contribution. A possible justification for neglecting s-d hybridization (the interaction of s and d functions where their energies cross) lies in the fact that in evaluating ϵ we are dealing with integral effects whereas the s-d interaction influences the s and d bands only in a relatively small range of $\vec{k}$ space.

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