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Microscopic Theory of Lattice Dynamics in Conducting Crystals*

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The microscopic formulation of lattice dynamics is examined in the long-wavelength limit for a general conducting crystal. Formulas for the elastic constants are derived for a complex metallic crystal.

I. INTRODUCTION

There have been an enormous number of investigations of the lattice dynamics of simple metals by the method of pseudopotentials. In this method, the crystal-structure effect is retained only in the direct ion-ion interaction; the electron screening is calculated in the homogeneous-electron-gas approximation. This approximation is not appropriate for more or less tightly bound electrons such as the d electrons in the noble metals, transition metals, and their intermetallic compounds. The general formulation of the ionic and electronic contribution to lattice vibrations in crystals has been given and the long-wavelength behavior for the insulating crystals has been examined.[1,2]

Here, we wish to investigate the long-wavelength behavior of phonons in a conducting crystal and derive the formulas for the elastic constants. In the following paper, we shall present an application of the formulation made here to a conducting crystal of some complexity, namely, intermetallic compounds of the Nb_3Sn type.

II. DYNAMICAL MATRIX AND ITS LONG-WAVELENGTH BEHAVIOR

In Refs. 1 and 2, the dynamical matrix has been given in terms of the microscopic interactions and response functions. We shall write it here in a form convenient for taking the small-wave-vector limit in metals.

Denote the equilibrium lattice vector by $\vec{x}_l$ and the equilibrium ion position in the unit cell by $\vec{x}_\kappa$. Thus, the equilibrium position of the $(l\kappa)$ ion is $\vec{x}_{l\kappa} = \vec{x}_l + \vec{x}_\kappa$. Let the charge and mass of the $(l\kappa)$ ion be $Z_\kappa e$ and M_κ. $-e$ is the charge of the electron.

The interaction potentials are (i) electron-electron: $v(r) = e^2/r$; (ii) ion-ion: $Z_\kappa Z_{\kappa'} v(r)$; and (iii) electron-ion: $v(\vec{r};\kappa)$. For large r, $v(\vec{r};\kappa) \sim -Z_\kappa v(r)$, but in the core region, we allow deviation of the ionic potential from the Coulomb potential. In actual computations, it is often convenient to account for the effects of core electrons by a pseudopotential. We may then regard $v(\vec{r};\kappa)$ as including the pseudopotential component in the core region.

The effective interaction between two ions of κ, κ' kind, respectively, at positions $\vec{x}$ and $\vec{x}'$ is

$$V(\vec{x}\kappa;\vec{x}'\kappa') = Z_\kappa Z_{\kappa'} v(\vec{x}-\vec{x}') + \int d\vec{r} \int d\vec{r}'\, v(\vec{x}-\vec{r};\kappa) \times \chi(\vec{r},\vec{r}') v(\vec{r}'-\vec{x}';\kappa') \quad , \tag{2.1}$$

where $\chi(\vec{r},\vec{r}')$ is the electron-density response function. The force constant for the two ions in the harmonic approximation is given by

$$\Phi_{\alpha\alpha'}(l\kappa, l'\kappa') = V_{\alpha\alpha'}(\vec{x}_{l\kappa}\kappa;\vec{x}_{l'\kappa'}\kappa') - \delta_{ll'}\delta_{\kappa\kappa'} \sum_{l''\kappa''} V_{\alpha\alpha'}(\vec{x}_{l\kappa}\kappa;\vec{x}_{l''\kappa''}\kappa'') \, , \tag{2.2}$$

where

$$V_{\alpha\alpha'}(\vec{x}\kappa,\vec{x}'\kappa') = \frac{\partial^2 V(\vec{x}\kappa;\vec{x}'\kappa')}{\partial x_\alpha \partial x'_{\alpha'}} \quad . \tag{2.3}$$

Hence, the dynamical matrix for phonons of wave vector $\vec{q}$ (restricted to the first Brillouin zone) is

$$\Phi_{\alpha\alpha'}(\vec{q};\kappa\kappa') = (M_\kappa M_{\kappa'})^{-1/2} \Omega_0^{-1} \times \sum_{\vec{G},\vec{G}'} [V_{\alpha\alpha'}(\vec{q}+\vec{G}\kappa;\vec{q}+\vec{G}'\kappa') - \delta_{\kappa\kappa'} \sum_{\kappa''} V_{\alpha\alpha'}(\vec{G}\kappa;\vec{G}'\kappa'')] \, , \tag{2.4}$$

where

$$V_{\alpha\alpha'}(\vec{q}+\vec{G}\kappa;\vec{q}+\vec{G}'\kappa') = e^{i(\vec{q}+\vec{G})\cdot\vec{x}_\kappa}(\vec{q}+\vec{G})_\alpha \times V(\vec{q}+\vec{G}\kappa;\vec{q}+\vec{G}'\kappa')(\vec{q}+\vec{G}')_{\alpha'} e^{-i(\vec{q}+\vec{G}')\cdot\vec{x}_{\kappa'}} \, . \tag{2.5}$$

$\vec{G}$ and $\vec{G}'$ are reciprocal-lattice vectors and Ω_0 is the unit-cell volume. $V(\vec{q}+\vec{G}\kappa;\vec{q}+\vec{G}'\kappa')$ is the double Fourier transform of the effective interaction $V(\vec{x}\kappa;\vec{x}'\kappa')$. Thus, from Eq. (2.1),

$$V(\vec{q}+\vec{G}\kappa;\vec{q}+\vec{G}'\kappa') = Z_\kappa Z_{\kappa'} v(\vec{q}+\vec{G})\delta_{\vec{G},\vec{G}'} + v(\vec{q}+\vec{G};\kappa) \times \chi(\vec{q}+\vec{G},\vec{q}+\vec{G}') v(-\vec{q}-\vec{G}';\kappa') \quad . \tag{2.6}$$

The Fourier transform $v(\vec{q}+\vec{G})$ of the Coulomb interaction is defined by

$$v(\vec{q}+\vec{G}) = 4\pi e^2/|\vec{q}+\vec{G}|^2 \quad \text{if } \vec{q}+\vec{G}\neq 0$$
$$= 0 \quad \text{if } \vec{q}+\vec{G}=0. \tag{2.7}$$

This takes care of the charge neutrality of the system.

We wish to investigate the phonon frequencies as $q \to 0$. Now, the dynamical matrix in Eq. (2.4) contains factors $v(q)$ which diverges as $q \to 0$. It is convenient to separate out such terms and exhibit them. Thus, we separate the Coulomb interaction into a long-range part $v(q)$ and a short-range part:

$$\hat{v}(\vec{q}+\vec{G}) = v(\vec{q}+\vec{G}) \quad \text{if } \vec{G}\neq 0$$
$$= 0 \quad \text{if } \vec{G}=0 \, . \tag{2.8}$$

A similar separation is made of the electron-ion potential.

Denote by $\hat{\chi}(\vec{q}+\vec{G},\vec{q}+\vec{G}')$ the sum of all polarization diagrams not containing the Coulomb term $v(\vec{q})$.[3] Then, $\hat{\chi}(\vec{q}+\vec{G},\vec{q}+\vec{G}')$ is well behaved as $q \to 0$. The limit does not necessarily vanish when $\vec{G}=0$ or $\vec{G}'=0$ in the case of conducting crystals.[4] This is quite different from the insulating crystals.[1]

We define a dielectric function $\epsilon(\vec{q})$ by

$$\epsilon(\vec{q}) = 1 - v(\vec{q})\hat{\chi}(\vec{q},\vec{q}) \, . \tag{2.9}$$

Then, the effective ion-ion interaction can also be separated as follows:

$$\begin{aligned}
V(\vec{q}\kappa;\vec{q}\kappa') &= v(q) + v(q;\kappa)[\hat{\chi}(\vec{q},\vec{q})/\epsilon(\vec{q})]v(\vec{q};\kappa') \, , \\
V(\vec{q}\kappa;\vec{q}+\vec{G}'\kappa') &= v(\vec{q},\kappa)\hat{\chi}(\vec{q},\vec{q}+\vec{G})v(\vec{q}+\vec{G}',\kappa')/\epsilon(\vec{q}) \, , \\
V(\vec{q}+\vec{G}\kappa;\vec{q}\kappa') &= v(\vec{q}+\vec{G},\kappa)\hat{\chi}(\vec{q}+\vec{G},\vec{q})v(\vec{q},\kappa')/\epsilon(\vec{q}) \, , \\
V(\vec{q}+\vec{G}\kappa;\vec{q}+\vec{G}'\kappa') &= \hat{V}(\vec{q}+\vec{G}\kappa;\vec{q}+\vec{G}'\kappa') \\
&\quad + v(\vec{q}+\vec{G};\kappa)\hat{\chi}(\vec{q}+\vec{G},\vec{q})[v(q)/\epsilon(\vec{q})] \\
&\quad \times \hat{\chi}(\vec{q},\vec{q}+\vec{G}')v(\vec{q}+\vec{G}';\kappa') \, .
\end{aligned} \tag{2.10}$$

The short-range part of the effective interaction $\hat{V}$ is obtained from the total interaction V by putting $v(\vec{q})$ to zero but keeping $v(\vec{q}+\vec{G})$.

By using Eqs. (2.10), we write the dynamical

matrix as

$$\Phi_{\alpha\alpha'}(\vec{q};\kappa\kappa') = (M_\kappa M_{\kappa'})^{-1/2}\Omega_0^{-1}\{e^{i\vec{q}\cdot\vec{x}_\kappa}q_\alpha[Z_\kappa Z_{\kappa'}v(q) - v(q;\kappa)v(q;\kappa')/v(q)]q_{\alpha'}e^{-i\vec{q}\cdot\vec{x}_{\kappa'}} + e^{i\vec{q}\cdot\vec{x}_\kappa}Z_\alpha^\dagger(\vec{q};\kappa)[v(q)/\epsilon(q)]Z_{\alpha'}(\vec{q},\kappa')e^{-i\vec{q}\cdot\vec{x}_{\kappa'}} + \sum_{\vec{G},\vec{G}'}[\hat{V}_{\alpha\alpha'}(\vec{q}+\vec{G}\kappa;\vec{q}+\vec{G}\kappa') - \delta_{\kappa\kappa'}\sum_{\kappa''}\hat{V}_{\alpha\alpha'}(\vec{G},\kappa,\vec{G}'\kappa'')]\} \quad . \quad (2.11)$$

In this way, we have separated out terms with short-range interaction which are well behaved as $q \to 0$ and terms which may possibly be of long range. $Z_\alpha(\vec{q},\kappa)$ is given by

$$Z_\alpha(\vec{q},\kappa) = -i[q_\alpha v(q;\kappa)/v(q) + \sum_{\vec{G}}\hat{\chi}(\vec{q},\vec{q}+\vec{G}) \times v(\vec{q}+\vec{G},\kappa)(\vec{q}+\vec{G})_\alpha e^{-i\vec{G}\cdot\vec{x}_\kappa}] \quad . \quad (2.12)$$

It may be regarded as the effective charge of the κ sublattice per unit displacement in α direction in a lattice vibration of wave vector $\vec{q}$.

Now, it is easy to examine the $q \to 0$ limit. For metallic crystals, because $\hat{\chi}(0,0)$ is finite, $\epsilon(q) \to \infty$ as $q \to 0$. The long-range interaction $v(q)$is screened to short range. The effective charge tends to

$$Z_\alpha(0;\kappa) = N^{-1}\int d\vec{r}\int d\vec{r}'\,\chi(\vec{r},\vec{r}') \times \sum_l\left(\frac{-\partial v(\vec{r}'-\vec{x}_{l\kappa};\kappa)}{\partial r'_\alpha}\right) \quad . \quad (2.13)$$

This is the change of the mean number of electrons per unit displacement of the sublattice κ. Therefore, it vanishes because of charge neutrality.

It follows that for conducting crystals, unlike insulators,

$$\lim_{q\to 0}\Phi_{\alpha\alpha'}(\vec{q};\kappa\kappa') = \Phi_{\alpha\alpha'}(0;\kappa\kappa') \quad . \quad (2.14)$$

Because all the long-range interactions are screened out in conductors, we have shown that the long-wavelength phonon frequencies tend to their zero-wave-vector value. In particular, the three acoustic branches tend to zero because of infinitesimal translational invariance which ensures that

$$\sum_{\kappa'}\Phi_{\alpha\alpha'}(0;\kappa\kappa') = 0 \quad . \quad (2.15)$$

III. ELASTIC CONSTANTS

We now derive formulas for the elastic constants of metallic crystals by the method of long waves.[5] That is, the elastic constants are determined from the sound velocities of acoustic phonons in the long-wavelength limit.

We follow Born and Huang[5] by expanding in powers of q the modified dynamical matrix

$$C_{\alpha\alpha'}(\vec{q};\kappa\kappa') = \Phi_{\alpha\alpha'}(\vec{q};\kappa\kappa')e^{-i\vec{q}\cdot(\vec{x}_\kappa-\vec{x}_{\kappa'})} \quad . \quad (3.1)$$

Consider first the "short-range" part in Eq. (2.11):

$$T_{\alpha\alpha'}(\vec{q};\kappa\kappa') = \Omega_0^{-1}\sum_{\vec{G},\vec{G}'}e^{-i\vec{q}\cdot(\vec{x}_\kappa-\vec{x}_{\kappa'})} \times\hat{V}_{\alpha\alpha'}(\vec{q}+\vec{G}\kappa;\vec{q}+\vec{G}'\kappa') \quad . \quad (3.2)$$

Then,

$$T_{\alpha\alpha'}(\vec{q};\kappa\kappa') = \sum_l e^{-i\vec{q}\cdot(\vec{x}_{l\kappa}-\vec{x}_{\kappa'})}\hat{V}_{\alpha\alpha'}(\vec{x}_{l\kappa}\kappa;\vec{x}_{\kappa'}\kappa') \quad . \quad (3.3)$$

The q expansion can be made directly from the Fourier transforms in Eq. (3.2) or from Eq. (3.3). In the latter case, we have

$$T_{\alpha\alpha'}(\vec{q};\kappa\kappa') = T^{(0)}_{\alpha\alpha'}(\kappa\kappa') + iq_\beta T^{(1)}_{\alpha\alpha',\beta}(\kappa\kappa') + \tfrac{1}{2}q_\beta q_{\beta'}T^{(2)}_{\alpha\alpha',\beta\beta'}(\kappa\kappa') + \cdots \quad , \quad (3.4)$$

with summation over repeated Greek indices understood:

$$T^{(0)}_{\alpha\alpha'}(\kappa\kappa') = \sum_l\hat{V}_{\alpha\alpha'}(\vec{x}_{l\kappa}\kappa;\vec{x}_{\kappa'}\kappa') \quad ,$$
$$T^{(1)}_{\alpha\alpha',\beta}(\kappa\kappa') = -\sum_l(x_{l\kappa\beta}-x_{\kappa'\beta})\hat{V}_{\alpha\alpha'}(\vec{x}_{l\kappa}\kappa;\vec{x}_{\kappa'}\kappa') \quad , \quad (3.5)$$
$$T^{(2)}_{\alpha\alpha',\beta\beta'}(\kappa\kappa') = -\sum_l(x_{l\kappa\beta}-x_{\kappa'\beta})(x_{l\kappa\beta'}-x_{\kappa'\beta'}) \times\hat{V}_{\alpha\alpha'}(\vec{x}_{l\kappa}\kappa;\vec{x}_{\kappa'}\kappa') \quad .$$

Separate the electron-ion potential into two parts:

$$v(\vec{q};\kappa) = -Z_\kappa v(\vec{q}) + v_R(\vec{q};\kappa) \quad . \quad (3.6)$$

$v_R(\vec{q};\kappa)$ is well behaved as $q \to 0$. Then, from Eqs. (3.1) and (2.11), a q expansion for the modified dynamical matrix gives the coefficients, defined in a similar way to Eq. (3.4), as follows:

$$C^{(0)}_{\alpha\alpha'}(\kappa\kappa') = (M_\kappa M_{\kappa'})^{-1/2}[T^{(0)}_{\alpha\alpha'}(\kappa\kappa') - \delta_{\kappa\kappa'}\sum_{\kappa''}T^{(0)}_{\alpha\alpha'}(\kappa\kappa'')] \quad , \quad (3.7)$$

$$C^{(1)}_{\alpha\alpha',\beta}(\kappa\kappa') = (M_\kappa M_{\kappa'})^{-1/2}T^{(1)}_{\alpha\alpha',\beta}(\kappa\kappa') \quad , \quad (3.8)$$

$$C^{(2)}_{\alpha\alpha',\beta\beta'}(\kappa\kappa') = (M_\kappa M_{\kappa'})^{-1/2}\{T^{(2)}_{\alpha\alpha',\beta\beta'}(\kappa\kappa') + (\delta_{\alpha\beta}\delta_{\alpha'\beta'}+\delta_{\alpha\beta'}\delta_{\alpha'\beta})[Z_\kappa v_R(0;\kappa') + Z_{\kappa'}v_R(0,\kappa)]\Omega_0^{-1} - [Z^{(1)}_{\alpha\beta}(\kappa)Z^{(1)}_{\alpha'\beta'}(\kappa') + Z^{(1)}_{\alpha\beta'}(\kappa)Z^{(1)}_{\alpha'\beta}(\kappa')]/\Omega_0\hat{\chi}(0,0)\} \quad . \quad (3.9)$$

The coefficients $Z^{(1)}_{\alpha\beta}(\kappa)$ are from the q expansion of the effective charge

$$Z_\alpha(\vec{q},\kappa) = iq_\beta Z^{(1)}_{\alpha\beta}(\kappa) + O(q^2) \quad . \quad (3.10)$$

The coefficient $C^{(2)}$, which contributes to the elastic constants, contains not only the contribution from the short-range force constants but also from the screened long-ranged interaction and from the $q \to 0$ limit of the deviation of the electron-ion potential from the Coulomb potential.

The eigenvalues of dynamical matrix determine

the squares of the phonon frequencies. As $q \to 0$, the eigenvalues for the acoustic branches are of the order q^2. We need to apply first-order perturbation theory to $C^{(2)}$ and second-order perturbation theory to $C^{(1)}$. By comparing the phonon equations to order q^2 with the equation of elastic waves,[5] we obtain the elastic constants

$$c_{\alpha\gamma,\beta\lambda} = [\alpha\beta, \gamma\lambda] + [\beta\gamma, \alpha\lambda] - [\beta\lambda, \alpha\gamma] + (\alpha\gamma, \beta\lambda) \quad , \tag{3.11}$$

with the equilibrium condition

$$[\beta\gamma, \alpha\lambda] = [\alpha\lambda, \beta\gamma] \quad , \tag{3.12}$$

where

$$[\alpha\beta, \gamma\lambda] = (2\Omega_0)^{-1} \sum_{\kappa\kappa'} (M_\kappa M_{\kappa'})^{1/2} C^{(2)}_{\alpha\beta\gamma\lambda}(\kappa\kappa') \tag{3.13}$$

and

$$(\alpha\gamma, \beta\lambda) = -\Omega_0^{-1} \sum_j [\omega(O_J)]^{-2} \times \Big[\sum_{\kappa\kappa'\alpha'} w_{\alpha'}(\kappa' \mid O_J) C^{(1)}_{\alpha'\alpha\gamma}(\kappa'\kappa) M_\kappa^{1/2}\Big] \times \Big[\sum_{\kappa''\kappa'''\alpha''} w_{\alpha''}(\kappa'' \mid O_J) C^{(1)}_{\alpha''\beta\lambda}(\kappa''\kappa''') M_{\kappa'''}^{1/2}\Big] \quad . \tag{3.14}$$

$\omega(O_J)$ and $w_\alpha(\kappa \mid O_J)$ denote the frequency and polarization vector of Jth optical mode at $\vec{q} = 0$.

When a complex crystal is subjected to a homogeneous strain, the sublattices may move relative to one another. $(\alpha\gamma, \beta\lambda)$ represents the contribution of such effects to the elastic constant. In Eq. (3.14), we have put it in a more explicit form than Born and Huang.[5]

In simple metals with one atom per unit cell and conduction electrons nearly free, some of the terms considered here are not important. For example, $(\alpha\gamma, \beta\lambda)$ vanishes. We shall see, however, in the following paper that for an intermetallic compound such as Nb_3Sn, careful inclusion of such terms from a general theory is essential to an understanding of its lattice dynamics and crystal instabilities.

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Theory of Lattice Dynamics of Nb_3Sn-Type Compounds*

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We present a method of calculating electron screening in the tight-binding approximation and constructing the dynamical matrix for the β-W compounds. We show that, in the cubic phase, no long-wavelength optical mode is temperature dependent except Γ_{12} which has a weak temperature variation. By the method of long waves, we calculate the elastic constants, particularly $c_{11} - c_{12}$, as a function of temperature, obtaining a fair agreement with experiment. We infer that the cubic to tetragonal phase transition is due to the instability of the $c_{11} - c_{12}$ shear mode, associated with which is a tetragonal distortion of Γ_{12} symmetry, in agreement with the neutron-scattering experiment of Shirane and Axe.

I. INTRODUCTION

A number of intermetallic compounds A_3B of β-tungsten (A-15) structure have very high superconducting transition temperatures and undergo a structural phase transition (from cubic to tetragonal) at low temperatures. These have been the subject of intensive experimental and theoretical investigations.[1]

The feature of interest to us here is the unusual temperature dependence of the phonon properties. The temperature dependence of the elastic constants has been measured for V_3Si,[2] V_3Ge,[3] and Nb_3Sn.[4,5] Neutron measurements have recently been carried out for V_3Si[6] and Nb_3Sn.[7,8] There also have been several calculations of the elastic constants[1,9-11] and the phonon frequencies.[12-14]

In this paper, we show how, given a tight-binding model for the d electrons, we can calculate from first principles the phonon spectrum (Sec. II). In particular, we give a careful treatment of the screening of the effective ion interaction by d as well as s electrons, in contrast to previous