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MODIFIED KREBS MODEL AND ITS APPLICATION TO fcc COBALT

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Résumé. — On a calculé, pour les principales directions de symétrie, les courbes de dispersion de phonons du cobalt en réseau à faces centrées suivant un modèle de réseau dynamique qui tient compte des interactions entre premiers voisins seulement. L’interaction electron-ion est décrite suivant le modèle proposé par Krebs. La pression ionique a été introduite pour maintenir l’équilibre du cristal. Les courbes déduites de ce modèle simple sont en accord avec les résultats expérimentaux.

Abstract. — Dispersion frequencies for face centred cobalt have been computed along the principal symmetry directions on the basis of a lattice dynamical model which takes into account central and angular interaction coupling with the first neighbours only. The electron-ion interaction has been described along the lines suggested by Krebs. Ionic pressure has been introduced to maintain the crystal equilibrium. The simple model gives a satisfactory explanation of phonon dispersion curves and a reasonably good agreement with measured data has been obtained.

1. Introduction. — Metallic crystals may be considered as multiparticle systems. Analysis [1, 2] of electron-gas energy leads to the conclusion that beside the central interactions between ions there exists an unpaired interaction via the conduction of three or more ions. This interaction plays a fundamental role particularly in the dynamics of vibrations and determines in particular the appearance of covalent type forces in a metal. Clark et al. [3] and de-Launay [4] proposed the existence of such forces under the name angular forces. Clark et al. (CGW) have studied the lattice dynamics of iron and vanadium and later a similar study was carried out by Yuen and Varshni [5] for the lattice vibrations in copper. Varshni and Yuen [6] have also described the role played by de-Launay (DAF) type angular forces in the lattice dynamical behaviour of copper.

The effect of conduction electrons was first considered by Fuchs [7] and later described by several authors [8-12]. All these studies suffer from three defects viz.

a) The electron-gas part of the dynamical matrix does not reproduce the periodicity of frequencies in reciprocal space.

b) The question of equilibrium of the whole lattice comprising ions and electrons has not been solved adequately.

c) The first-order term in the expression of the electron-energy has not been considered properly.

The electron-ion interaction reported by Krebs [13] and Cheveau [14] satisfies the symmetry requirement but the derivative of the screened Coulombian interaction-energy in the Krebs model is not zero at equilibrium (Cochran [15]). Some of the recent studies [16, 17, 18] have considered the effect of electron-pressure in maintaining the lattice-stability. The study due to Das et al. [16] evaluates electronic volume strain at ionic sites which is questionable. The other studies [17, 18] have shown that only the kinetic part of the electron-energy goes to develop the electron pressure.

In the present communication, the total interaction governing the lattice vibrations in fcc cobalt is taken to consists of four parts i.e.

a) A radial-interaction (second derivative of the coupling potential) among nearest neighbour ions.

b) A transversal-interaction (first derivative of the coupling potential) between the nearest neighbour ions, which develops the ionic pressure.

c) A CGW type angular interaction coupling the nearest neighbours only and

b) A radial-interaction (second derivative of the coupling potential) among nearest neighbour ions.

The screening-effect of conduction electrons limits the ion-ion interaction to nearest neighbours only. Further the ionic pressure balances the electron pressure and thus the lattice stability is preserved.

The model has been employed to compute the
phonon-frequencies for the cobalt, which undergoes a
first-order martensitic phase transformation from a
high temperature face-centred cubic (fcc) structure
to a hexagonal closed packed (hcp) structure at
\( T \sim 420 ^\circ \text{C} \). A pure single crystal of fcc cobalt has
not been studied experimentally to date because of
two facts. First, the 420 \(^\circ\)C phase transformation is
very unstable and secondly cobalt is a strong neutron
absorber. However it can be understood that alloying
the cobalt with small concentrations of similar
structures like Fe or Ni does not change its fcc
structure significantly. Recently Shapiro and Moss [19]
have measured the phonon-energies of an alloy
\( \text{(Co}_{0.92}\text{Fe}_{0.08}) \) which could be identified as a close
approximation to fcc cobalt. The model yields the
phonon-frequencies which are shown to be in good
agreement with those derived from the experimental
phonon-energies [19].

2. Formulation and results. — The usual secular
determinant expressing the phonon-frequencies \( (v) \)
may be written as

\[
| D(q) - 4 \pi^2 m v^2 I | = 0 \tag{1}
\]

where \( m \) is the mass of the ion and \( I \) is the unit matrix
of order three. The elements of the dynamical matrix
\( D(q) \) are the sum of the following two terms:

\( a) \) the ion-ion terms \( D^I(q) \) and

\( b) \) the ion-electron terms \( D^E(q) \).

The ion-ion contribution to the dynamical matrix i.e.
\( D^I(q) \) may be written as the sum of two terms, one due
to central interactions \( (D^{IC}(q)) \) and the other due to
angular interactions \( (D^{IA}(q)) \) coupling the nearest
neighbours. The expressions for \( D^{IC}(q) \) and \( D^{IA}(q) \)
may be written following Maradudin et al. [20] and
Yuen and Varshni [5] respectively as

\[
D^{IC}(q) = 4(\beta_1 + 2 \alpha_1) - 2(\beta_1 + \alpha_1) c_x(c_y + c_z) - 4 \alpha_1 c_y c_z \tag{2}
\]

\[
D^{IA}(q) = 4(\beta_1 - \alpha_1) s_x s_y \quad \text{(fcc)}
\]

and

\[
D^{IA}(q) = 32 K_1 - 16 K_1 c_y c_z - 4 K_1(2 c_{2x} - c_{2y} - c_{2z}) \tag{3}
\]

\[
D^{IA}(q) = - 16 K_1 s_x s_y \quad \text{(fcc)}
\]

where \( \alpha, \beta = x, y, z ; s_x = \sin(q_x l) ; c_x = \cos(q_x l) \).

\( c_{2x} = \cos(q_x l) \). \( a \) is the lattice constant and \( q_x \)
is the \( x \)-component of the phonon wave vector \( q \). \( K_1 \)
the angular force parameter. \( \alpha_1 \) and \( \beta_1 \) are respectively
the first and the second derivatives of the central
potential \( \phi \) coupling the nearest neighbour ions i.e.

\[
\alpha_1 = \frac{\partial \phi(r)}{\partial r} \left( \frac{1}{r} \right) \right) \tag{4}
\]

Considering the crystal structure as comprising of
electrons located in the uniform background of
positive charges, we can write the practical constraint
governing the lattice equilibrium as

\[
P_1 = P_e \tag{5}
\]

where \( P_1 \) is the ionic pressure and \( P_e \) is that due to
electrons responding to the ionic motion. Obviously

\[
P_1 = \frac{\partial \phi}{\partial \Omega} \quad \Omega \text{ is the atomic volume} \tag{6}
\]

Using equations (5) and (6) we arrive at the result:

\[
\alpha_1 = \frac{a}{4} P_e \tag{7}
\]

Substituting this value of \( \alpha_1 \) in equation (2) and
adding the resultant to equation (3), we may write the
final expression for the element \( D^I(q) \) as:

\[
D^I(q) = 4 \left( \beta_1 + \frac{a}{2} P_e + 8 K_1 \right) - 2 \left( \beta_1 + \frac{a}{4} P_e + 8 K_1 \right) c_y(c_x + c_z) - a P_e c_y c_z - 4 K_1(2 c_{2x} - c_{2y} - c_{2z}) \tag{8}
\]

\[
D^I(q) = 2 \left( \beta_1 - \frac{a}{4} P_e - 8 K_1 \right) s_x s_y \quad \text{(fcc)}
\]

We can write the electron-ion contribution \( (D^{IE}(q)) \) following Krebs [13] as

\[
D^{IE}(q) = A \sum_{\text{h}} \left[ \frac{(q + h)_x (q + h)_y g^2((q + h) | r_x) - h_x h_y g^2((h | r_x)}{(q + h)^2 + \lambda^2 f(t_1)} \right] \tag{9}
\]
where \( h \) is the reciprocal lattice vector, \( r_i \) is the radius of the Wigner-Seitz sphere, and \( \lambda \) is the screening parameter [21] i.e.

\[
\lambda = 0.353(r_0/a_0)^{1/2} K_F
\]  

(10)

where \( r_0 = r_s/Z^{1/3} \) is the electronic spacing, \( K_F \) is the radius of the Fermi-sphere, \( Z \) is the valence and \( a_0 \) is the Bohr-radius.

The function \( f(t) \) is given by the expression

\[
f(t) = 0.5 + \frac{1 - t^2}{4 t} \ln \left( \frac{1 + t}{1 - t} \right),
\]

(11)

where \( A \) is a constant which depends on the effective charge on the ions and the Wigner-Seitz factor

\[
g(x) = 3(\sin x - x \cos x)/x^3 \quad \text{(Wigner-Seitz)}. \quad (12)
\]

Three of the four model parameters \((aP_e, \beta_1, K_1, A)\) are evaluated by expanding equation (1) in the long wavelength limit and comparing to Christoffel's [22] equation of elasticity. This comparison leads to the following elastic relations.

\[
\begin{align*}
ac_{11} &= 2 \beta_1 + \frac{a}{2} P_e + 32 K_1 + 4 A/a^2 \lambda^2 \\
ac_{12} &= \beta_1 - \frac{5}{4} aP_e - 16 K_1 + 4 A/a^2 \lambda^2 \\
ac_{44} &= \beta_1 + \frac{3}{4} aP_e
\end{align*}
\]

(12)

The fourth model parameter is evaluated by knowing a zone boundary frequency for a transverse mode along the [001] direction. The required equation may be expressed as

\[
4 \pi^2 m v_f^2 [100] = 4 \beta_1 + 3 aP_e + 32 K_1 + D_{pF}(q_{max}).
\]

(13)

It may be noted the set of equations (12) show an equivalence with those derived on the basis of homogeneous deformation theory [23]. The relations (12) used for evaluating the model parameters are consistent with the condition of zero initial stress playing a key role in the methods of long wave [24] and homogeneous deformation [25] for the components of the elastic constant tensor. A similar consistency is contained in equation (13).

The input data and the computed model parameters for fcc cobalt are shown in Table I.

3. Discussion. — It may be mentioned that the phenomenological models reported so far describe in general the lattice equilibrium somewhat superficially. They all equate the ionic and electronic pressures separately to zero. The present communication deals with possible practical equilibrium condition represented by equation (5). The Cauchy discrepancy as outlined by the present model may be written as

\[
ac_{12} - ac_{44} = \frac{4 A}{a^2 \lambda^2} - 2 aP_e - 16 K_1.
\]

(14)

Obviously the long range \((4 A/a^2 \lambda^2)\) and short range \((2 aP_e)\) electron response to the ionic motion contributes significantly to the anisotropy exhibited by the crystal. A part of it is certainly attributed to the threebody interaction denoted by \( K_1 \).

The computed phonon-frequencies for the fcc cobalt are shown in figure 1. The frequencies, derived from experimental phonon-energies are shown by circles and triangles. The good agreement between the theoretical and experimental data suggests that the simple model can describe the lattice dynamical behaviour of a somewhat complicated structure like that of the fcc cobalt.

![Dispersion frequencies for fcc cobalt along the symmetry directions. Continuous line (—) shows the computed frequencies, circles and triangles (○) denote the experimental ones derived from the phonon-energies reported by Shapiro and Moss [19].](image)

**FIG. 1.** — Dispersion frequencies for fcc cobalt along the symmetry directions. Continuous line (—) shows the computed frequencies, circles and triangles (○) denote the experimental ones derived from the phonon-energies reported by Shapiro and Moss [19].

**Table I**

**Input data and computed model parameters for fcc cobalt**

<table>
<thead>
<tr>
<th>Input data</th>
<th>Ref.</th>
<th>Computed model parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_{11} )</td>
<td>( 2.21 \times 10^{12} ) dynes/cm^2</td>
<td>( aP_e = 4.749 \times 10^4 ) dynes/cm</td>
</tr>
<tr>
<td>( c_{12} )</td>
<td>( 1.47 \times 10^{12} ) dynes/cm^2</td>
<td>( \beta_1 = 0.839 \times 10^4 ) dynes/cm</td>
</tr>
<tr>
<td>( c_{44} )</td>
<td>( 1.24 \times 10^{12} ) dynes/cm^2</td>
<td>( K_1 = 0.135 \times 10^4 ) dynes/cm</td>
</tr>
<tr>
<td>( a )</td>
<td>( 3.55 ) Å</td>
<td>( A = 16.039 \times 10^4 ) dynes/cm</td>
</tr>
<tr>
<td>( m )</td>
<td>58.7 amu</td>
<td></td>
</tr>
<tr>
<td>( v_T )</td>
<td>( 5.87 \times 10^{12} ) Hz</td>
<td></td>
</tr>
</tbody>
</table>
References