Crystal Equilibrium and Lattice Dynamical Study of α-Iron and Chromium

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Studies of the phonon dispersion, the temperature dependence of Debye-Waller factor, the Debye temperature, and the mean square displacement of α-iron and chromium have been made by means of a lattice dynamical model proposed by the authors. The model considers short range pairwise forces effective up to the second neighbours and electron-ion interactions on the lines of Bhatia using an appropriate value of the screening parameter. The volume force is averaged over the whole Wigner-Seitz sphere. The ionic lattice is in equilibrium in a medium of electrons. The computed results compare well with experimental data.

1. Introduction

During the last two decades, several attempts[1-5] have been made to study the lattice dynamics of cubic metals using realistic models on a first principles approach. The task, however, remains formidable. Normally, phonon spectra have been analyzed on the lines of the Born-Kármán theory of lattice vibrations[6]. This requires a large number of force constants to be used as independent parameters[7,8], a proper physical interpretation of which can not be given. Therefore, efforts[9-12] have been made to develope elastic force models in which the nature and magntiude of the forces between the free electrons and the ions are accounted for reasonably. These models have been excellently reviewed by Joshi and Rajagopal[13]. In this review article, a very important point concerning the crystal equilibrium has been overlooked. In the models of de Launay[9], Sharma and Joshi[11], and Krebs[12], the crystal lattice is in equilibrium for the central forces alone. Equilibrium conditions for the model solid have not been imposed by these authors, and hence their claim about the magnitude of the Cauchy discrepancy is erroneous. Furthermore, they assume that in equilibrium the derivatives of the potential energy for each set of neighbouring ions (i.e. α_j) are individually zero; in addition to this, they also neglect the electronic pressure. In this context, Thomas[14] stressed that the energy terms and hence their first derivatives cannot be set separately euqual to zero in an equi-

librium configuration. He emphasized that an elastic constant theory only applies to a solid in equilibrium and that an equilibrium condition must be imposed explicitly for empirical models for lattice cohesion. Thus, in equilibrium the algeberic sum of the pressures due to the ionic potential and the electron gas must vanish, i.e.

$$p_0^i + p_0^e = 0, \qquad (1)$$

where the subscript 0 refers to the equilibrium configuration.

In the present paper, we have developed a phenomenological model which considers ion-ion interactions through a second neighbor pair potential[15] and electron-ion interactions on the lines of Bhatia using a realistic value of the screening parameter. The volume force has been averaged over the whole Wigner-Seitz sphere. The proposed model is in equilibrium under zero external stress and gives the correct expression for the Cauchy discrepancy. The electron-ion interaction part of the dynamical matrix following Bhatia's approach is rigorous, based on sound physical grounds, and easy to compute as evidenced by the published work[16,17]. The proposed model has been used to study the phonon dispersion in three major symmetry directions, the temperature variation of the Debye-Waller factor, the Debye characteristic temperature, and the mean square displacement for α-iron and chromium.

2. The Model

The system in which the vibrations take place consists of point ions, having their equilibrium positions at the lattice points, and of an electron gas surrounding the ions. The assumption of point ions

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is valid for most of the simple [18] and transition cubic [5] metals excepting Group-IB metals. The phonon frequencies in the harmonic approximation are given by the secular equation:

$$| D_{12}(\boldsymbol{q}) - M \omega_q^2 \delta_{12} | = 0, \quad \mu = 1, 2, 3 \tag{2}$$

where $\quad D_{12}(\boldsymbol{q}) = D_{12}^{i-i}(\boldsymbol{q}) + D_{12}^{i-e}(\boldsymbol{q})$. $\tag{3}$

Here the $D_{12}(\boldsymbol{q})$ are the elements of the dynamical matrix, $\boldsymbol{q}$ is the wave vector confined to the first Brillouin zone (BZ), and M is the mass of the ion.

Following Maradudin et al. [15], the ion-ion contribution to the dynamical matrix for bcc structures is given by the following expressions:

$$D_{11}^{i-i} = \tfrac{8}{3}(2\alpha_1 + \beta_1)(1 - C_1 C_2 C_3)$$
$$+ 4\beta_2 S_1^2 + 4\alpha_2 (S_2^2 + S_3^2), \tag{4}$$
$$D_{12}^{i-1}(\boldsymbol{q}) = \tfrac{8}{3}(\beta_1 - \alpha_1) S_1 S_2 C_3, \tag{5}$$

where α_1, α_2, β_1, and β_2 are the pair potential force constants, S_μ and C_μ are $\sin(\pi a k_\mu)$ and $\cos(\pi a k_\mu)$, respectively, and $q_\mu = 2\pi k_\mu$. Here we have confined the ion-ion interaction upto second nearest neighbours only, as the bare electron ion interaction reduces the effect of long range coulomb interactions to short range forces between ions [2]. The merit of this procedure has very recently been enumerated by Upadhyay [19], who has shown that the central pairwise potential [15] stands on sound theoretical grounds and that the angular force models produce no additional results and create confusion. Further, Bertoni et al. [20] have also shown that central pairwise interactions between ions give a good description of the lattice dynamics of cubic metals.

Bhatia's approach provides an electron-ion contribution to the dynamical matrix of the form

$$D_{12}^{i-e} = \frac{4\pi e n' K_e q_1 q_2 \Omega}{4\pi e n' + |\boldsymbol{q}|^2}, \tag{6}$$

where $n' = (4\pi m e/h^2)(3\pi)^{1/3} n_0^{1/3}$. Here m is the electronic mass, e the electronic charge, n_0 the average density of the electron, and h Planck's constant. The modified form of the electronic part of the dynamical matrix is

$$D_{12}^{i-e} = \frac{K_e q_1 q_2 \Omega}{1 + (q^2/\lambda^2)} G^2(q r_0). \tag{7}$$

Here the original model of Bhatia has been modified in the following way:

(i) Bhatia's theory considers the force at the centre of the ion. Here, we have averaged the force

over the whole Wigner-Seitz sphere. This gives the term $G^2(q r_0)$ in Eq. (7), where

$$G^2(x) = \left[\frac{3(\sin x - x \cos x)}{x^3} \right]^2 \tag{8}$$

and $x = q r_0 = q r_e/Z^{1/3}$ (Raimes [21]). Here r_0 is the interelectronic spacing, r_e the radius of the Wigner-Seitz sphere, and z the chemical valence.

(ii) Bhatia's approach to calculate the Thomas-Fermi screening parameter in terms of the elastic constants of the metal is erroneous [22]. Therefore, we have replaced the term $4\pi e n'$ by λ^2 known as the screecing parameter given by

$$\lambda^2 = \lambda^2(P) f(t), \tag{9}$$

where $\quad \lambda(P) = 0.353 (r_0/a_0)^{1,2} k_F$ $\tag{10}$

and

$$f(t) = \tfrac{1}{2} + \frac{1 - t^2}{2t} \ln \left| \frac{1+t}{1-t} \right| \tag{11}$$

with $t = k/2 k_F$. Here a_0 is the Bohr radius and k_F the Fermi surface wave vector. The function $f(t)$ in Eq. (9) has been included since the screening parameter $\lambda(P)$ in a high density electron gas is k dependent [23]. The screening parameter $\lambda(P)$ has been borrowed from Pines [24].

The potential energy U of the crystal is the sum of the potential energies $U^i \left(= \sum_j U_j^i \right)$ and U^e corresponding to the ion-ion and electron-ion interactions, respectively. The lattice equilibrium is determined by the vanishing of the total pressure independent of direction i.e. $(\partial U^i/\partial \Omega) a + P^e = 0$, where the electronic pressure $P^e = \partial U^e/\partial \Omega$ is assumed to be isotropic. Writing

$$\alpha_j = \frac{1}{r_j} \left(\frac{\mathrm{d}U^i}{\mathrm{d}r_j} \right) \text{and} \quad P^e = \frac{3}{5} K_e$$

for free electrons [9,10], the equilibrium condition assumes the following form:

$$\alpha_1 + \alpha_2 + \tfrac{3}{10} a K_e = 0. \tag{12}$$

A large number of solid state phenomena such as neutron scattering, Mössbauer effect, electrical conductivity, melting of crystals etc. are governed by an exponential factor e^{-2W}, often called Debye-Waller (DW) factor. The DW factor $2W$ is assumed to consist of two parts: (a) The phonon dependent part W', which is obtained from the knowledge of the whole vibration spectrum. (b) The part W'',

which is the contribution of the central part of the Brillouin zone, corresponding to $q = 0$ and is evaluated in the Debye approximation.

(a) Following James [25] and a recent paper of one of us [26] we can write

$$2\,W' = \frac{8\,\pi^2\,\hbar}{3\,m\,N}\left(\frac{\sin\theta}{\lambda}\right)^2 \sum_{q,j}\frac{1}{\omega_{q,j}}\,\mathrm{Coth}\left(\frac{\hbar\,\omega_{q,j}}{2\,k_{\mathrm{B}}\,T}\right) \quad (13)$$

where m is the mass of the atom, N the total number of unit cells in the crystal, $\omega_{q,j}$ the angular frequency of phonon wave vector q with polarization j, $e_{q,j}$ the polarization vector of (q, j) lattice mode, $\hbar$ Plancks constant divided by 2π, k_{B} the Boltzmann constant, T the absolute temperature, θ the glancing angle, and λ the wavelength of the incident radiation, and the summation extends over all the normal vibrations of the crystal.

(b) Since all the modes are acoustic for a monatomic lattice, ω is zero when $q = 0$. Following Barron and Smith [27], we can avoid this singularity in the sum by replacing the contribution to the sum at $q = 0$ with an integration of the energy term, $(E/4\pi^2\nu^2$ (of the mode of lattice vibrations))

$$E = \hbar\,\omega\,[\{\exp(\hbar\,\omega/k_{\mathrm{B}}\,T) - 1\}^{-1} + \tfrac{1}{2}] \quad (14)$$

over a sphere of volume equal to 20^{-3} of the Brillouin zone near $q = 0$. It is assumed that the frequency is given in this region by the average velocity times the wave-vector. The zero phonon contribution W'' is then written as

$$W'' = \frac{a^3}{3\,m}\,\{D(C_{\mathrm{L}}) + 2\,D(C_{\mathrm{T}})\}\left(\frac{\sin\theta}{\lambda}\right)^2, \quad (15)$$

where

$$D(C) = \frac{1}{C^2}\int_0^{2\pi k_{\max}} 4\,\pi^2\,\hbar\,C\,k\,\mathrm{d}k$$
$$\times\left[\left\{\exp\left(\frac{\hbar\,\omega}{k_{\mathrm{B}}\,T}\right) - 1\right\}^{-1} + \frac{1}{2}\right]. \quad (16)$$

C_{L} is the average velocity for the longitudinal phonons and C_{T} is that for the transverse phonons in this region. $k_{\max}$ is the radius of the sphere of integration and is given by

$$\frac{4\,\pi}{3}\,k_{\max}^3 = 20^{-3}\ (\text{volume of the Brillouin zone})$$

or $\quad k_{\max} = \dfrac{1}{20\,a}\left(\dfrac{3}{2\,\pi}\right)^{1/3}$ (for bcc) metals. (17)

$D(C)$ can be reduced to

$$D(C) = P\left(\frac{1}{x}\int_0^x\frac{t\,\mathrm{d}t}{e^t - 1}\right) + \frac{1}{4}\,P\,x, \quad (18)$$

where

$$P = \frac{4\,\pi^2\,k_{\mathrm{B}}\,T\,k_{\max}}{C^2}\ , \quad x = 4\,\pi^2\,\hbar\,k_{\max}\,C/k_{\mathrm{B}}\,T$$

and $t = (2\,\pi\,\hbar\,k\,C/k_{\mathrm{B}}\,T)$.

The value of the integral contained in the expression for $D(C)$ can be substituted from standard tables. The Debye-Waller factor W is now calculated from the equations (13) and (15). For a Debye model of the solid, the temperature dependence of the Debye-Waller exponent can be written as

$$2\,W = 48\,\pi^2\,\hbar^2\,T/m\,k_{\mathrm{B}}\,\Theta_{\mathrm{M}}^2\,\{\Phi(x) + x/4\}\,(\sin\theta/\lambda)^2. \quad (19)$$

Here Θ_{M} represents the effective x-ray characteristic temperature, $\Phi(x)$ the usual Debye integral function and $x = \Theta_{\mathrm{M}}/T$.

Similarly, in harmonic approximation, the mean square displacement of the atoms $\bar{u}^2$ is given by the following relation

$$\bar{u}^2 = \frac{3}{8\,\pi^2}\left(\frac{\lambda}{\sin\theta}\right)^2\cdot W\,. \quad (20)$$

3. Numerical Computation

The three equations of elastic constants and one equilibrium condition equation (12) together with one zone boundary frequency in [100] direction form necessary set of equations to determine five parameters of the theory. The remaining four equations are as follows:

$$a\,C_{11} = \tfrac{2}{3}\,(2\,\alpha_1 + \beta_1) + 2\,\beta_2 + a\,K_{\mathrm{e}}\,, \quad (21)$$

$$a\,C_{12} = \tfrac{2}{3}\,(\beta_1 - 4\,\alpha_1 - 3\,\alpha_2) + a\,K_{\mathrm{e}}\,, \quad (22)$$

$$a\,C_{44} = \tfrac{2}{3}\,(2\,\alpha_1 + \beta_1) + 2\,\alpha_2\,, \quad (23)$$

$$m\,\pi^2\,\nu_{\mathrm{T}}^2 = \tfrac{4}{3}\,(2\,\alpha_1 + \beta_1)\,. \quad (24)$$

The input data for finding the above force constants and their calculated values for α-iron and chromium is given in Table 1. These force constants are used to calculate the phonon dispersion relations along the three major symmetry directions.

The Debye-Waller exponent $2\,W$ for α-iron and chromium have been calculated by the Blackmann's root sampling technique [28]. For this purpose it is essential to determine the vibration frequencies at a suitable number of points in an irreducible section

Table 1. Input parameters and calculated force constants.

| | C_{11} | C_{12} | C_{44} | Lattice parameter Å | Density gm/cm^{-3} | Temp. (K) | $v_T(100)$ | Source | α_1 | α_2 | β_1 | β_2 | αK_e |
	All in units of 10^{12} Dyn. cm^{-2}								All in units of 10^3 Dyn. cm^{-1}				
α-iron	23.31	13.55	11,78 [a]	2.8662	7.87	300	8.52	Ref. [33]	−0.9634	0.2752	51.7563	15.6463	2.2941
Chromium	35.00	6.78	10.08 [b]	2.8792	7.19	298	7.83	Ref. [43]	−0.1581	1.4541	39.4995	39.4989	−4.32

[a] J. A. Rayne and B. S. Chandrasekhar, Phys. Rev. 122, 1714 [1961].
[b] D. I. Bolef and J. de Klerk, Phys. Rev. 129, 1063 [1963].

of the first Brillouin zone. In order to keep the frequencies within limits and yet to have a fairly large sample, we have considered a mesh of 8000 wave vectors evenly distributed in the first Brillouin zone. From the symmetry requirements the eight thousand points were reduced to 256 non-equivalent points, including the origin, lying within 1/48 irreducible part of the Brillouin zone.

The secular equation determining the lattice frequencies of the metals was solved for these non-equivalent points, and thus the complete vibrational spectrum was obtained. In evaluating the summation in Eq. (13), we divided the whole vibrational spectrum into a number of frequency intervals and assigned appropriate weights to each interval. The mean square displacement of the atoms $\bar{u}^2$ and the Debye characteristic temperature Θ_M at different temperatures were evaluated from Eqs. (20) and (19), respectively.

4. Comparison with Experiments

The calculated and experimental dispersion curves along three symmetry directions for α-iron and chromium are presented in Figures 1 and 2. The comparison of the calculated and experimental Debye-Waller factors may be made in terms of a temperature parameter Y defined by

$$Y = \log_{10} e \, (\lambda/\sin\theta)^2 \, (2\,W_{T0} - 2\,W_T),$$

where W_{T0} and W_T are the Debye-Waller exponents at the temperatures T_0 and T, respectively. This quantity is independent of λ and θ and is directly accessible from the measured x-ray intensities of the Bragg reflections,

$$I_T/I_{T0} = \exp(-2\,W_T)/\exp(-2\,W_{T0}),$$

where I_T and I_{T0} are the x-ray intensities at temperatures T and T_0, respectively. Hence, we have $Y = (\lambda/\sin\theta)^2 \log_{10}(I_T/I_{T0})$. The calculated values of Y, $\bar{u}^2$, and Θ_M at different temperatures for α-iron and chromium are presented in Figs. 3 and 4, respectively. For comparison, the corresponding values deduced from various x-ray measurements have also been plotted.

α-iron

The phonon dispersion of α-iron has been experimentally studied through inelastic neutron scattering techniques by many workers [29-36]. Early work on the lattice dynamics of α-iron by Curien [29]
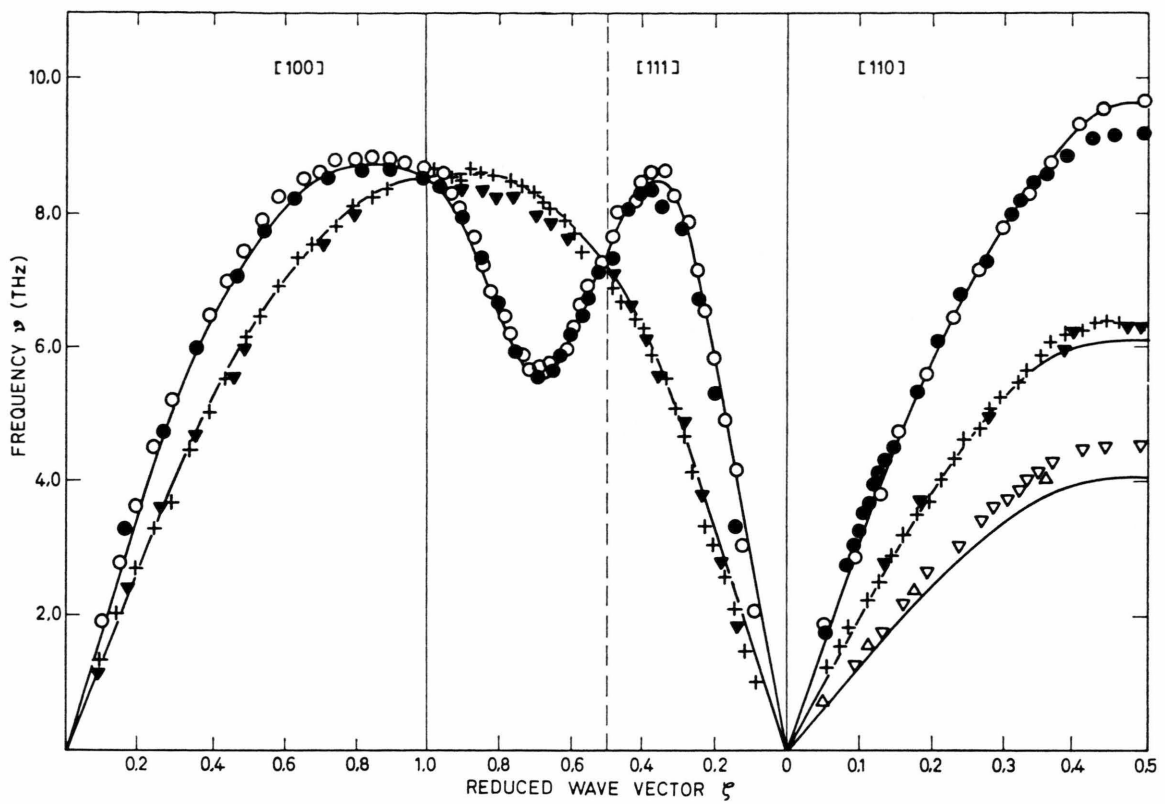
Fig. 1. Dispersion curves along symmetry directions for α-iron. Solid curves correspond to present calculations. Experimental points: ●▼△ Minkiewics et al.; ○+▼ Bergsma et al.
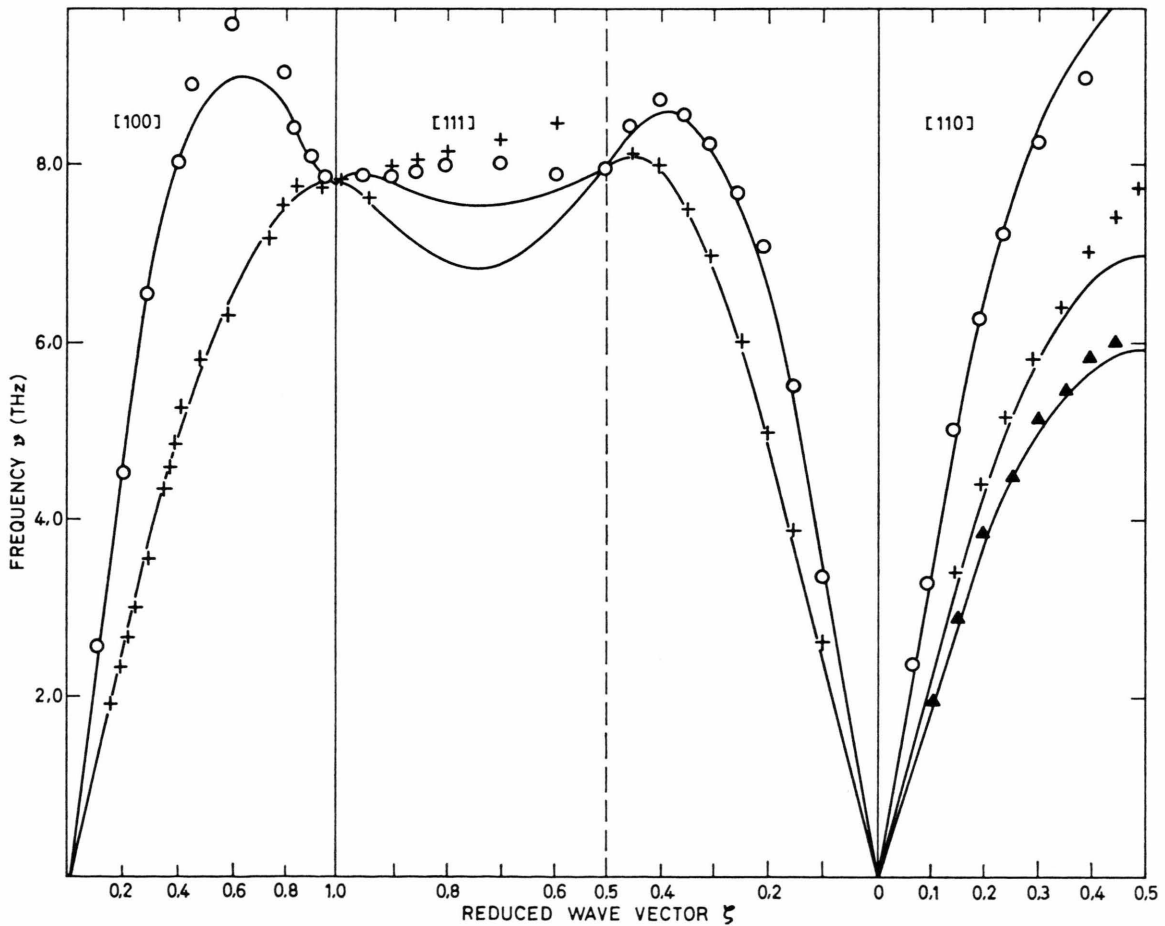

Fig. 2. Dispersion curves along symmetry directions for Chromium. Solid curves correspond present calculations. Experimental points: ○+▼ Shaw and Muhlestein.

using diffuse X-ray scattering and by Iyenger et al.[30] using inelastic neutron scattering was relatively poor and did not give sufficient information. The measurements of Low[31] using neutron time of flight techniques are also incomplete and somewhat uncertain; no data are given for the longitudinal and transverse branches with the polarization vector normal to the (110) plane in [110] direction. Brockhouse et al.[32] have reported more complete results along the main symmetry directions at 296 K. Recently Minkiewics et al.[33], Bergsma et al.[34], and Schweiss et al.[35] have made a detailed study of the phonon dispersion in α-iron at 295 K for the phonon wave vector along the three symmetry directions. The measurements of Minkiewicz et al. agree well with those of Brockhouse et al. but are in serious disagreement with those of Bergsma et al. for the longitudinal mode near the zone boundary in [110] direction. The results of Minkiewicz et al. also differ appreciably from those of van Dingenen and Hautecler[36] on α-iron crystal containing 3.5% silicon. For the present comparison, the values obtained from the measurements of Minkiewicz et al. and Bergsma et al., as these extend over the entire Brillouin zone, are plotted in Fig. 1 along with our theoretical ones. The overall agreement is quite satisfactory.

The effect of the temperature variation of the Debye-Waller factors for α-iron has been studied by both x-ray diffraction (Ilyine and Kritskaya[37], Haworth[38], Herbstein and Smuts[39], and γ-ray resonant absorption experiments (Debrunner and Morrison[40]). The x-ray measurements of Haworth covered the temperature range $286-1190$ K by making integrated intensities and peak height measurements of the diffraction line (220) for an iron spectrum. The results show large scatter associated with crystal changes brought about by prolonged annealing. The observed x-ray intensities for iron by Ilyina and Kristakaya and by Herbstein and Smuts refer to room temperature only and are therefore not selected for the present comparison. The experimental data of Haworth are plotted in Fig. 3 along with a few experimental measurements of Debrunner and Morrison in the temperature range $293-573$ K. The theoretical results agree reasonably well with the experiments upto 1000 K. Above this temperature, the observed decrease in the intensity of the reflections becomes greater than that expected theoretically.
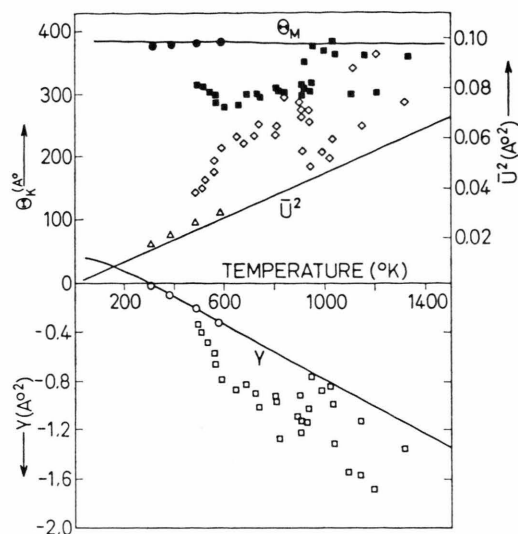

Fig. 3. Variation of y, $\bar{u}^2$, and Θ_M with temperature for α-iron. Solid curves show present calculations. Experimental points: $\square$, $\diamondsuit$, $\blacksquare$ Haworth; $\circ$, $\triangle$, $\bullet$ Debrunner and Morrison.

Chromium:

Möller and Mackintosh[41] have measured phonon dispersion curves of chromium by neutron scattering technique. Due to the relative sparseness of the data these dispersion curves did not receive much attention, however an analysis in terms of the fourth neighbor Born-Karman model has been done by Feldman[42]. Shaw and Muhlestein[43] have measured detailed phonon dispersion curves of chromium at room temperature in the three symmetry directions by means of thermal neutron scattering. These phonon dispersion relations show four regions of anomalous behaviour. The experimental data along with our theoretical ones are plotted in Fig. 3. A reasonably satisfactory agreement between theory and experiment is observed.

Reliable integrated x-ray intensity data for single crystals of chromium at different temperatures have been reported by Wilson et al.[44] in the temperature range $100\,K < T < 520\,K$. The data were corrected for thermal diffuse scattering as well as changes in the lattice parameters. The authors have expressed their results in terms of a characteristic Debye temperature. For comparison's sake, we have calculated the quantity $(\lambda/\sin\theta)^2 \log_{10} e(I_T/I_0)$ as a function of temperature from the corresponding values of the Debye temperatures. Ilyina and Kristkaya[37] have also reported measurements of the x-ray Debye temperature of chromium, but their
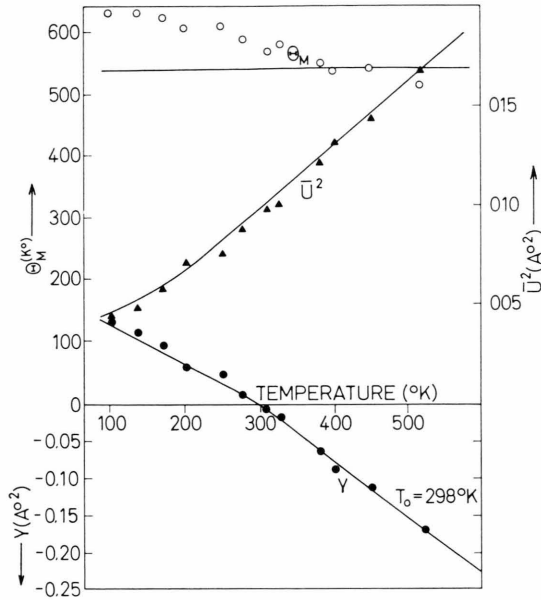
Fig. 4. Variation of y, $\bar{u}^2$, and Θ_M with temperature for chromium. Solid curves show the present calculations. Experimental points: ●, ▲, ○ Wilson et al.

measurements are confined to room temperature only. The values of Y, Θ_M, $\bar{u}^2$ deduced from the measurements of Wilson et al. are plotted in Fig. 4, with $T_0 = 293$ K. The theoretical Y values are in satisfactory agreement with the experimental data, but the $\Theta_M - T$ curves show large deviations in the theoretically and experimentally determined values. The marked discrepancy may partly be attributed to the uncertainty in the determination of integrated intensities, and it appears that some other factor predominates in the case of chromium.

5. Discussion

Our dispersion curves are in better agreement with the experiments than the theoretical calculations of Cavalheiro and Shukla [45] for α-iron, and of Pal [46] for chromium.

However, in the recent past various phenomenological models have been used by a number of workers [46-51] to compute the exponent $2W$ using their vibration spectra. In summing the series, the term corresponding to $k = 0$ has been neglected by these workers, because the value of the wave-vector in this case corresponds to a non-vibrating lattice for which the DW exponent vanishes. Therefore, the

contribution of the central part of the Brillouin zone has not been taken into account in these calculations and much reliance cannot be bestowed upon their computed $2W$ values.

Important features of ion-electron-ion interaction, such as Kohn anomalies and Fredel oscillations associated with the Fermi surface have been left out in the present study. Anharmonic effects have also been ignored. The incomplete d-electronic shells responsible for the large cohesive energy [52] in transition metals are also expected to make an important contribution to the forces governing the lattice vibrations.

The DW factor temperature parameter Y offers a satisfactory explanation for the observed temperature variation of the x-ray intensities of Bragg reflections upto a certain temperature. At higher temperatures, the experimental values of $2W$ are consistently higher than the theoretical ones, and this discrepancy increases with temperature. The disagreement between theory and experiment at high temperatures may be attributed to the neglect of lattice expansion (Zener and Bilinsky [53] and other anharmonic effects (Hahn and Ludwig [54], Cowley [55], Maradudin and Flinn [56], Slater [57], Wolfe and Goodman [58], and Willis [59]). Anharmonic contributions vary mostly as the square of the absolute temperature and become predominant at high temperatures. In the calculations no account has been taken of the temperature variation of the elastic constants and the lattice parameter. With the increase in temperature, the normal mode frequencies are decreased because of thermal expansion. This effect depends upon the Grüneisen parameter, which changes with lattice frequencies and temperature. According to studies made by various workers it has been seen that the frequency distributions of fcc metals can be approximated by two peaks, the lower frequency peak being of larger area. At higher temperatures, the Debye-Waller exponent depends upon the lattice frequencies as $\sum_{q,j} \omega_{q,j}^{-2}$. The lower frequency peak therefore contributes much more to $2W$ than the higher frequency peak and therefore largely governs the intensity of the x-ray reflections. Since the Grüneisen parameter of this peak and its temperature variation is not known, no quantitative claculation of the thermal expansion effect on the x-ray intensities has been possible.

Thus, we would like to enumerate additional advantages of the present scheme:

1. The model satisfies the equilibrium condition under zero external stress.

2. Equations (22) and (23) give the Cauchy discrepancy in the form:

$$C_{12} - C_{44} = -4(\alpha_1 + \alpha_2) + a K_e .$$

which can be written in view of the equilibrium condition (12) as $C_{12} - C_{44} = 2.2 K_e$.

3. Earlier models[9, 11, 12] neglect the pressure due to the electron gas and assume the first derivative of the potential energy for each set of neighboring ions to be zero individually. In our model, the derivative of the total potential energy is taken to be zero.

In conclusion, we can say that the present model explains most of the lattice dynamical properties of α-iron and chromium satisfactorily.

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