Ashcroft model potential study of lattice dynamics of α-Iron and barium

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Ashcroft model potential has been used to compute phonon dispersion relations along the three principal symmetry directions, *i.e.* [k00], [kk0] and [kkk] for α-iron and barium. The computed phonons gave a reasonable agreement with the experimental ones in all the three principal summetry directions expect for the T_2 branch in [KK0] direction where the present study failed to reproduce the experimental findings.

Keywords: Ashcroft potential; lattice dynamics; α-iron; barium

Se ha empleado el modelo de potencial de Ashroft para evaluar las relaciones de dispersión de fonón para α-acero y bario en tres direcciones principales de simetría: [k00], [kk0] y [kkk]. Los fonones evaluados coincidieron razonablemente con los obtenidos experimentalmente en las tres direcciones principales, excepto para la rama T_2 en la dirección [KK0], donde el presente estudio no ha reproducido los resultados experimentales.

Descriptores: Potencial de Ashroft; dinámica de redes; α-acero; bario

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1. Introduction

Both α-iron and barium belong to the body centered cubic structure. These metals are quite complicated with regard to their electronic structure as they posses a *spd* hybridisation with a part of the d band unfilled. While α-iron is a transition metal, barium is a heavy rare earth metal. For both of these metals experimental measurements on phonon dispersion relations have been carried out. Also a number of theorical studies of lattice dynamics of these metals are available on various forms of pseudopotentials. In the present work we have studied the lattice dynamics of these two metals on a very simple form of Ashcroft potential. The reasons to carry out such a work was motivated by the following:

- Ashcroft potential is well accepted for eletronic properties of almost all cubic metals. The lattice dynamical study of this potential has been carried out only for alkali metals (Ashcroft [1] and Sen *et al.* [2]).
- Ashcroft potential has only one adjustable parameter, the core radius. We adjusted this core radius with the experimental phonon of the one of the wave vectors lying in the bondary of the Brillouin zone.
- We wanted to know if lattice dynamics of a complicated metal like barium and α-iron could be studied by Ashcroft potential.

The frequency of vibration of a monoatomic lattice is obtained by solving the secular determinant

$$||D_{\alpha\beta}(\vec{q}) - m\omega^2 I|| = 0, \tag{1}$$

where $\vec{q}$ is the phonon wave vector, m is the ionic mass, I is the 3×3 unit matrix and ω is the angular frequency. Each element $D_{\alpha\beta}(\vec{q})$ is splited up into three parts, *i.e.*,

$$D_{\alpha\beta}(\vec{q}) = D^C_{\alpha\beta}(\vec{q}) + D^R_{\alpha\beta}(\vec{q}) + D^E_{\alpha\beta}(\vec{q}). \tag{2}$$

$D^C_{\alpha\beta}(\vec{q})$ is the direct coulomb interaction between ions, $D^R_{\alpha\beta}(\vec{q})$ is the core-core exchange repulsion and $D^E_{\alpha\beta}(\vec{q})$ is the electron ion interaction. In the present study $D^C_{\alpha\beta}(\vec{q})$ has been calculated on the lines of Kellerman [3]. We have ignored $D^R_{\alpha\beta}(\vec{q})$ in the present study. The electronic contribution to dynamical matrix is obtained by

$$D^E_{\alpha\beta}(\vec{q}) = \frac{N}{\Omega_0 m}\sum_{\vec{g}}[(\vec{q}+\vec{h})_\alpha(\vec{q}+\vec{h})_\beta F(|\vec{q}+\vec{h}|) - (\vec{h})_\alpha(\vec{h})_\beta F(|\vec{h}|)]. \tag{3}$$

$F(q)$ is the wave number characteristic defined by

$$F(q) = -\frac{\Omega_0 q^2}{8\pi Z e^2}|w_b(q)|^2\frac{\epsilon^*(q)-1}{[1-G(q)]}, \tag{4}$$

$\vec{h}$ are reciprocal lattice vectors, n is the number of ions in the primitive cell, Z is the valence of the ion and Ω_0 is the atomic

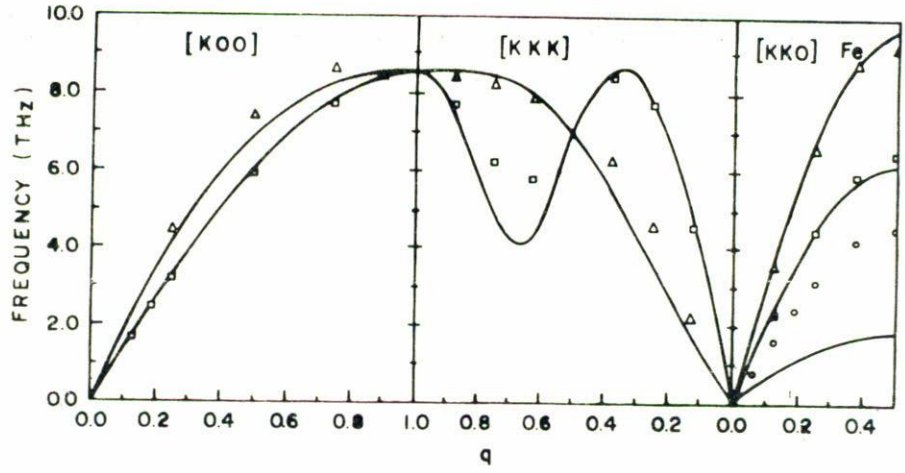

FIGURE 1. Phonon dispersion relations of α-iron along the three principal symmetry directions. Solid curves represent the computed results. Experimental points are shown by the symbols ○, Δ and □.

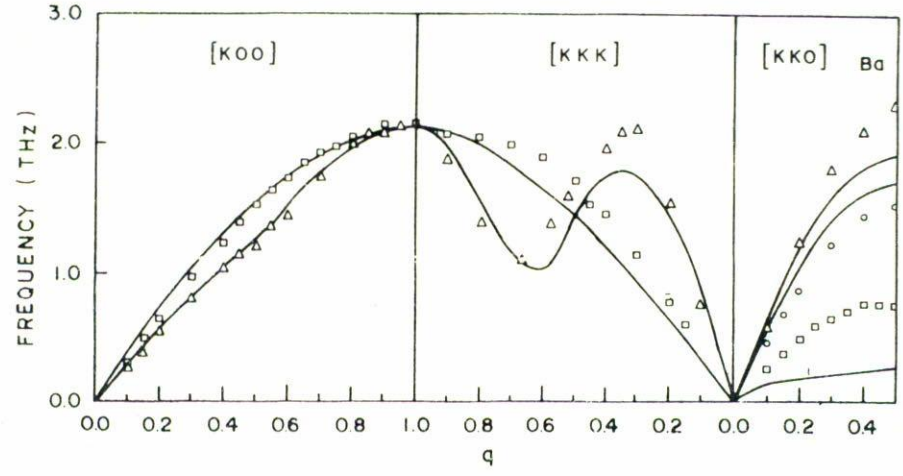

FIGURE 2. The same text as Fig. 1, but for barium.

volume, $w_b(q)$ is the Fourier transform of the Ashcroft model potential, given by

$$w_b(q) = -\frac{4\pi Z q^2}{\Omega_0 q^2}\cos(qr_c) \tag{5}$$

and $G(q)$ is due to Singwi *et al.* [5] by the expression

$$G(p) = \frac{9}{32}\left(\frac{q}{k_F}\right)^2\left[\frac{2}{105}\left(24\left(\frac{k_F}{q}\right)+44+\left(\frac{q}{k_F}\right)^2\right)\right.$$
$$-\frac{2k_F}{q}\left(\frac{8}{35}\left(\frac{q}{k_F}\right)^2-\frac{4}{15}+\frac{1}{6}\left(\frac{q}{k_F}\right)^2\right)ln\left|\frac{q+2k_f}{q-2k_f}\right|$$
$$\left.+\left(\frac{q}{k_F}\right)^2\left(\frac{1}{210}\left(\frac{q}{k_F}\right)^2-\frac{2}{15}\right)\ln\left|\frac{q^2-4k_F^2}{q^2}\right|\right].$$

The proper convergence for the summation in Eq. (3) has been obtained after summing 1178 reciprocal lattice vectors. We fitted the r_c with the longuitudinal zone boundary frequency $L_{1,0,0}$ for both α-iron and barium. The calculated value of r_c for barium is 2.01 (a.u.) and for α-iron is 1.16 (a.u.).

We solved the dynamical matrix (1) for several wave sectors along the principal symmetry directions and plotted the phonon dispersion relations along these directions in α-iron and barium in Figs. 1 and 2, respectively. Also in these figures are plotted the experimental phonon frequencies of α-iron by the work of Brookhouse *et al.* [4] and of barium by Mizuki *et al.* [5].

A critical observation of Figs. 1 and 2 reveals that the lattice dynamical study of α-iron and barium by Ashcroft model potential gave an excellent agreement with the experimental

findings. Except for T_2 branch of [k,k,0] reproduced the experimental results within an error of 9%. For barium also the computed curve does not reproduce the T_2 branch of [k,k,0]. In other two directions *i.e.* [k,0,0] and [k,k,k] the theorical result deviate by maximum by 12% of the experimental result for some of the wave vectors. Also the anomaly, the lowering of the longitudinal branch in [k,0,0] is well explained by this model.

There is no justification in comparing our theoretical study of α-iron with the earlier studies of Animalu [6], Onwagba [7] and Nagara and Nakamura [8] and Boselli *et al.* [9] and that of barium by Gupta *et al.* [10], Chen *et al.* [11], Wang and Overhouser [12] and Moriarty [13]. All these workers have used at least two parameters in pseudopotentials, exception of Moriarty whose work is from first principles, and their results are not superior to the present results.

If one asks us how such a simple model like that of Ashcroft gave a good description of the lattice dynamics of a *d* band metal like α-iron and barium, we would not be able to respond well. We can only say that probably the value of r_c barium and α-iron determined by us is responsible for this fact. Who knows the value of rc of α-iron and barium determined by us may be low or high as given by other physical properties of these metals. But as far knowledge goes there is no value quoted in the literature. What is more important is that we have been able to reproduce the experimental phonon frequencies of α-iron and barium on one parameter.

We can add here that we also tried to study the lattice dynamics of other b_{cc} transitions metals, molybdinum, tungsten, neobium, tantalum on Ashcroft model potential but with no success. The other rare earth metal of *bcc* structure *i.e.* strontium did not also give a good fit with the experimental phonons.

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