Indian J. Phys. **67A** (2), 145-148 (1993)

Phonons in fcc strontium

D Singh and R P S Rathore
Department of Physics, R B S College, Agra-282 002, India

Received 26 March 1992, accepted 11 June 1992

Abstract : A more realistic model, requiring a few parameters to explain the interactions among distant neighbours and valid to various crystallographic structures, is developed to study the phonon dispersion in *fcc* metals The model, free from usual fitting procedure, is employed to obtain phonon dispersion in *fcc* strontium, which has attracted scant attention so far The computed results showing good agreement with the recent experimental findings lend reliability and credibility to the theory

Keywords : Realistic model parameters, phonon dispersion, *fcc* strontium, ionic and electronic interactions

PACS No. : 63 20 Dj

1. Introduction

The macroscopic lattice dynamical studies usually employ increasing number of parameters to achieve credible success in their objective. No single model is equally efficable [1] in explaining the phonon dispersion in crystal of same structure, test to say of different structures. The recourse to common fitting procedure makes the model inadequate [2] and error prone [3]. Fielek [4] has pointed out the usual long wave elastic relations oftenly used for parameter evaluation ignore the Umklapp and volume-dependent screening terms.

The widely used [5-7] and exponential [8-10] potentials embody deficient [11, 12] behaviour at small separations.

The first principle computations due to Moriarty [13] and dynamical pseudopotential results of Wang and Overhauser [14] on *fcc* strontium are left uncompared with the neutron scattering data on the metal.

Present study is devoted to develop a more sound which dispels the said inconsistencies regarding its behaviour and the evaluation process. The computed phonon dispersion along the major symmetry directions of *fcc* strontium are compared with the recent experimental findings due to Buchenau *et al* [15].

The details of ionic and electronic interaction are out lined in Section 2. Section 3 deals briefly with the computations. The salient features of the present study are given in the last concluding section.

2. Formalism

2.1. The ionic interactions :

The generalised exponential potential incorporating the repulsive and attractive characters of the interaction is corrected for its proper behaviour at small separations. The factor r_j^{-1} rectifies the potential for this effect. The modified form of the potential assumes the form

$$\phi^I(r_j) = D\,[2(m-1)]^{-1} \sum_j r_j^{-1} [\exp\{-m\alpha(r_j - r_o)\} - m \exp\{-\alpha(r_j - r_o)\}] \qquad (1)$$

where D is the dissociation parameter, α the hardness parameter and r_o the equilibrium separation parameter. The exponent m provides for the appropriate adjustment of depth and width of the potential and implies the electronic exchange and correlation effects in an alternative and simple manner. The element of dynamical matrix having explicit bearing on eq. (1) may be written as

$$D_{xx}^I(q) = 4(\alpha_1 - \beta_1)[1 - 1/2\, C_{1x}(C_{1y} + C_{1z})] + 2(\alpha_2 - \beta_2)(1 - C_{2x}) + 4\beta_1[3 - (C_{1x}C_{1y} + C_{1y}C_{1z} + C_{1z}C_{1x})] + 2\beta_2[3 - (C_{2x} + C_{2y} + C_{2z})]$$

$$D_{xy}^I(q) = 2(\alpha_1 - \beta_1) S_{1x} S_{1y}$$

where $\alpha_1 = (\partial^2\phi^I/\partial\gamma_j^2)_N$, $\alpha_2 = (\partial^2\phi^I/\partial\gamma_j^2)_{NN}$

$\beta_1 = [1/\gamma_j (\partial\phi^I/\partial\gamma_j)]_N$, $\beta_2 = [1/\gamma_j (\partial\phi^I/\partial\gamma_j)]_{NN}$

$N \rightarrow$ Nearest neighbour, $NN \rightarrow$ next nearest neighbour

and $C_{1x} = \mathrm{Cos}(aq_{x/2})$, $C_{2x} = \mathrm{Cos}(aq_x)$

$S_{1x} = \mathrm{Sin}(aq_{x/2})$, $S_{2x} = \mathrm{Sin}(aq_x)$

q_x is the x ($= x, y, z$) component of phonon wave vector $\boldsymbol{q}$.

2.2. The electronic interaction .

The elements of dynamical matrix corresponding to electron-ion interactions are expressed on the lines of Oli [16]. The dielectric screening due to Shaw [17] is forged to achieve the correct convergence of the expression.

The total dynamical matrix [$= D_{xx}^I(q) + D_{xy}^E(q)$] is fed to the usual secular equation to obtain the phonon dispersion along the major symmetry directions in *fcc* strontium.

3. Computations

The procedure due to Girifalco and Weizer [18] is adopted to evaluate the parameter D, α and r_o. Present study consider the atoms extending out to eighth neighbour to compute these parameters. The criterion for lattice stability is integrated with the process of parameter evaluation. The needed input data and the corresponding computed parameters for the *fcc* strontium are given in Table 1. Table 2 records the evaluated derivatives α_1, α_2, β_1 and β_2 for the metal. Figure 1 shows the dispersion relation for the *fcc* strontium.

Table 1. Input data and computed defining parameters of *fcc* strontium

Input data		Computed defining parameters
Lattice constant	= 6.047 Å	$D = 1.2286268 \times 10^{-20}$ erg-cm
Cohesive energy	= 1.72 ev/atom	$\alpha = 0.81842$ Å^{-1}
Inverse compressibility	= 0.116×10^{12} dyne/cm^2	$r_0 = 5.27225$ Å

Table 2. Computed constants (α_1, α_2, β_1 and β_2) for the *fcc* strontium (10^4 dyne/cm).

α_1	β_1	α_2	β_2
0.477994	−0.04527	−0.002228	0.0070139

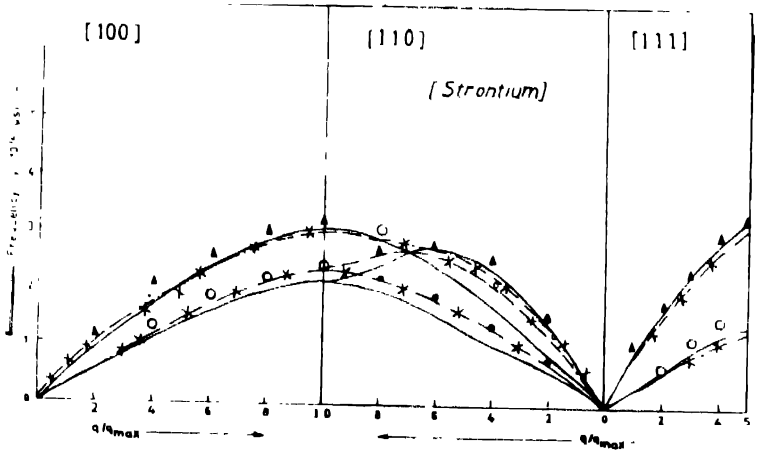

Figure 1. Phonon dispersion in the *fcc* strontium
(——·——) Present study
(▲○●) Experimental finding due to Buchenau *et al* [15]
(–× ×–) Theoretical prediction due to Singh and Rathore [9].

4. Conclusion

Present study endorses the following salient features :

(a) The study employs only two input data beside the lattice constant. This feature makes the study to excel over the pseudo model potential studies, which invariably require more than two input data to account for the interaction comprehensively.

(b) The study accounts,for the repulsive interactions in an consistent and less parametric manner. The recent model potential studies,either use additional Born-Mayer [7] potential or extra input data to accommodate these interactions. The older models however, ignore the interactions altogether.

(c) The study avoids the usual fitting procedure, a common feature of the

phenomenological studies. The study abandons the use of measured data on elastic constants (general statistical data) and phonon frequencies (essential dynamical data) in its evaluation procedure.

(d) The potential depicts the realistic features of the interactions in general and at small separations in particular.

(e) The potential is aptly corrected for the electronic exchange and correlation effects in a simple and meticulous manner.

(f) Present theory commands the inclusion of interaction to any distant neighbour without adding to any extra parameter. The usual macroscopic models require two fold additional parameters for the purpose.

(g) The potential beside being capable of explaining the ionic interactions for all the solids of a particular crystallographic structure, is generally adoptable for the metals of different structures [19-21]

Present study, being first of its kind predicts adequately the phonon dispersion in the *fcc* strontium, showing good agreement with the experimental findings due to Buchenau *et al* [15]. The results due to Singh and Rathore [9] are also compared for establishing the efficacy of the present theory.

References

[1] M Singh 1984 *Indian J Phys* **58A** 106

[2] P S Lay, B Szigette and V K Tewari 1971 *Proc Roy Soc* **A320** 505

[3] S K Sarkar, S K Das, D Roy and S Sengupta 1977 *Phys Stat Solidi (b)* **83** 613

[4] B L Fielek 1984 *J. Phys* **F14** 61

[5] B N Onwuaga 1987 *Phys Stat Solidi (b)* **105** 141, 1988 *Nuovo Cim* **D10 277**

[6] D Prakash and J C Upadhyaya 1988 *Phys Stat Solidi (b)* 148, K-109; 1988 *J Phys. Chem Solids* **49** 91

[7] M Born and J F Mayer 1932 *Z Phys* 75 1

[8] F Milstein 1975 *J Appl Phys.* **44** 3825, 3833

[9] G Singh and R P S Rathore 1986 *Phys. Stat Solidi (b)* **136** 57

[10] K Mohammed, M M Shukla, F Milstein and J L Merz 1985 *Phys Rev* **B29** 3117

[11] F R Dobbs and G O Jones 1957 *Rep Prog Phys* **20** 516

[12] K P Thakur 1974 *J Inorg. Nucl Chem* **36** 2171, 1976 *J Inorg Nucl. Chem* **38** 1433

[13] J A Moriarty 1983 *Phys Rev* **B28** 4818

[14] Y R Wang and A W Overhauser 1987 *Phys. Rev* **B35** 501

[15] U Buchenau, M Heiroth and H R Schober 1984 *Phys Rev* **B31** 3502

[16] B A Oli 1978 *J. Phys.* **F8** 2441

[17] R W Shaw 1970 *J Phys* **C3** 1140

[18] A Ginfalco and V G Weizer 1959 *Phys Rev* **114** 687

[19] Km Aradhana and R P S Rathore 1990 *Czec J. Phys* **B40** 686

[20] R P S Rathore, A Singh and R M Agrawal 1991 *Phys Stat Solidi (b)***165** 95

[21] R M Agrawal, Km Aradhana and R P S Rathore 1991 *Indian J. Pure Appl. Phys* **29** 517.