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The Lattice Dynamics and The Elastic Behaviour of fcc and bcc Ba

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Abstract

The two-body pairwise E.G.E.P. (Extended Generalized Exponantial Potential) type Morse potential and volume dependent energy are assumed to represent the total energy of the Ba crystal. The parametrized potential is used to calculate the second- and third-order elastic constants C_{ij} and C_{ijk}, pressure derivatives of bulk moduli and Grüneisen parameter γ. The phonon frequencies are also computed and plotted. The obtained results are compared with available experimental data and, in general, the agreement is good.

1. Introduction

Alkaline earth metals exhibit a number of interesting properties. The most striking one is the variety of crystal structures. At room temperature and normal pressure the stable structure is bcc for Ba. Phase transitions can also be induced by pressure. For the heavier elements of this group, e.g. Ca, Sr, and Ba, the situation is somewhat complicated by the presence of an empty d band just above the Fermi Level. For quantitative tests of theoretical calculations, the lattice dynamics is a useful tool since it contains detailed information and can be calculated easily by any familiar methods. Phonon dispersion curves of bcc Ba were determined experimentaly for the first time by U. Buchenau et al [1].

The pairwise(e.g. Morse or Rydberg type) potential model is not adequate, so in this study, the two-body pairwise E.G.E.P. (Extended Generalised Exponantial Potential) type Morse potential proposed by Verma and Rathore[2] plus a volume dependent energy ($\sum_n P_n V^n$) are assumed to represent the total enegy of Ba crystal. This total energy is applied to the second- and third-order elastic constants (C_{ij}, C_{ijk}) , pressure derivatives of elastic constants, pressure derivative of bulk modulus, Grüneisen parameter and phonon frequencies for fcc and bcc Ba.

2. Computational Procedure and Applications

The total interaction energy used in this work is assumed to be expressed by

$$\phi(r) = \frac{D}{(m-1)}[\, e^{-m\,\alpha\,(r-r_o)}/(\alpha\, r)^n - m\,(\alpha\, r)^n e^{-\alpha\,(r-r_o)}\,] + \sum_n P_n V^n, \qquad (1)$$

where D, α and r_o have their usual meanings. The parameter n appearing in(1) does not account explicitly for the three-body interactions but its presence in the potential function implicitly introduces the three- body character as stated by Verma [2]. The potential parameter D, α and r_o are calculated following the procedure given by Girifalco and Weizer[3]. For the volume dependent energy term, $(\sum_n P_n V^n)$, we choose n=1, and P_1 is evaluated using the procedure given by Najafabadi [4]. Input parameters are presented in Table 1. The calculated values of D, α and r_o and P_1 for fcc Ba and bcc Ba are listed in Table 2.

Table 1. Input Data [5].

Metal	Lattice Constants (A)	Cohesive Energy (eV/atom)	Bulk Modulus 10^{12} N/m^2
fcc Ba	6.31005	1.90	0.103
bcc Ba	5.00000	1.90	0.105

Table 2. The Computed Potential Parameters.

Metals	m	n	$\alpha(A^{-1})$	r_o(A)	D(erg)	P_1(dyn/cm^2)
fcc Ba	1.05	0.5	0.739138	8.533380	8.56164x10^{-15}	-0.30539x10^9
bcc Ba	0.5	0.5	1.355316	2.659295	5.27898x10^{-12}	-0.57487x10^9

3. Elastic Constants and Related Properties

Second- and third-order elastic constants, at atmospheric pressure and 0 K, are evaluated adopting the general expressions given by Born [6]. At T=0 K, the calculated values of the elastic constants are given in Table 3.

The hydrostatic pressure derivatives of second-order effective elastic constants are computed in terms of second- and third-order elastic constants by using the fallowing formula [7]:

$$\frac{\partial\, c'_{11}}{\partial\, P} = -(\frac{2c_{11} + 2c_{12} + c_{111} + 2c_{112}}{c_{11} + 2c_{12}}) \qquad (2)$$

$$\frac{\partial\, c'_{12}}{\partial\, P} = -(\frac{-c_{11} - c_{12} + c_{123} + 2c_{112}}{c_{11} + 2c_{12}}) \qquad (3)$$

$$\frac{\partial\, c'_{44}}{\partial\, P} = -(\frac{-c_{11} - 2c_{12} + c_{44} + 2c_{144} + 2c_{166}}{c_{11} + 2c_{12}}) \tag{4}$$

Table 3. The Calculated Two- and Third- Order Elastic Constants in Units of x10 ^{11} dyn/cm^2.

	fcc Ba	bcc Ba	
	This work	This work	Experiment (293K)[1]
C_{11}	1.213035	1.293198	1.0±0.3
C_{12}	0.881489	0.610789	0.642±0.2
C_{44}	0.51486	0.658536	0.95±0.05
C_{111}	-11.20019	-20.90064	
$C_{112} = C_{166}$	-5.58522	-3.684452	
$C_{123} = C_{456} = C_{144}$	-1.854586	-3.26945	

Also, the pressure derivative of Bulk modulus[8] and the Grüneisen parameter [9] are computed from the usual equations:

$$\frac{\partial B}{\partial P} = 1 - \frac{r_0}{3}\left[\frac{\frac{\partial^3\phi}{\partial r^3}}{\frac{\partial^2\phi}{\partial r^2}}\right] \text{ and } \gamma = -\frac{a}{6}\frac{(\frac{d^3\phi}{da^3})_{a=a_o}}{(\frac{d^2\phi}{da^2})_{a=a_o}} \tag{5}$$

and the obtained results are given in Table 4.

Table 4. Some Elastic Properties for fcc Ba and bcc Ba

Metals	$\frac{\partial C'_{11}}{\partial P}$	$\frac{\partial C'_{12}}{\partial P}$	$\frac{\partial C'_{44}}{\partial P}$	$\frac{\partial B}{\partial P}$	γ Cal.	Exp.[10]
fcc Ba	6.10937	5.08047	3.203665	4.17977	1.17564	—
bcc Ba	9.72713	4.98745	2.995430	2.73316	0.81467	0.721

4. Phonon Dispersion Curves

For potential function in Eq.(1), the phonon frequencies are calculated in usual manner for fcc and bcc Ba by solving the secular determinant

$$|\, D_{\alpha,\beta}(q) - Im\omega^2\,| = 0, \tag{6}$$

where m is ionic mass, ω is the angular frequency and I is unit matrix. Assumming the interaction forces effective up to third-nearest neighbour for Eq.(1), the calculated force constants (α angular force constants, β radial force constants) are given in Table 5. The obtained results for the phonon frequencies of fcc and bcc Ba in the principal symmetry directions are plotted in Figure 1 a and b, respectively.

Table 5. Calculated Force Constants in units dyn/cm.

Metals	α_1	α_2	α_3	β_1	β_2	β_3
fcc Ba	4981.791	67.296	-26.777	-513.041	72.228	4.7174
bcc Ba	6428.389	2886.077	-100.022	-515.490	-67.226	38.4425

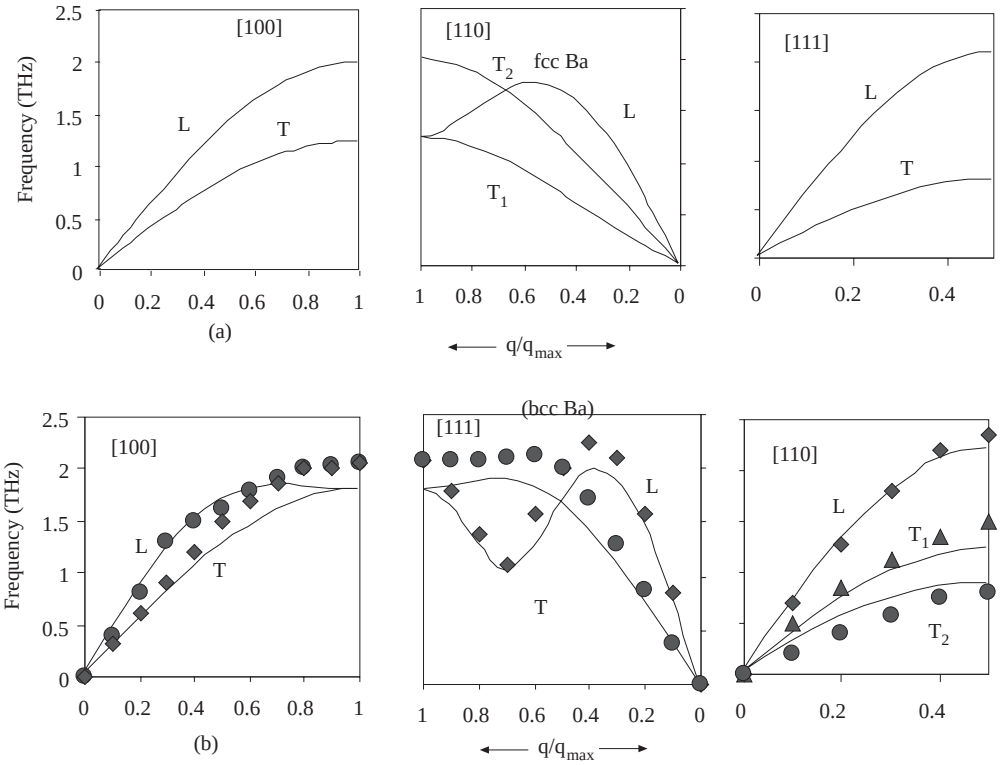

Figure 1. Phonon Dispersion Curves for a) fcc Ba and b) bcc Ba

5. Results and Discussion

The obtained phonon frequencies by using the E.G.E.P. function for bcc Ba are, generally, in agreement with the experimental data. The experimental findings for fcc Ba are not available, therefore we have compared our results with those computed by Moriarty[11]. The phonon frequencies for fcc Ba, except for $T[100]$ and $T_1[110]$ transverse branches of fcc Ba, are generally in agreement with Moriarty's data.

It can be seen from Table 3 that the computed values of SOEC for bcc Ba are in good agreement with that observed experimentally (no experimental data for TOEC for bcc phase). We belive that the volume dependent energy added to the two-body potential

has improved the present results.

To our knowledge, this is first calculations of pressure derivatives of elastic constants, pressure derivative of bulk modulu for Ba and, unfortunately, no experimental data are available for comparison.

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