Turkish Journal of Physics

Volume 24 | Number 2 Article 6

1-1-2000

The Lattice Dynamics of bcc Titanium

KEMAL ÇOLAKOĞLU

YASEMİN ÖZTEKİN ÇİFTÇİ

Turk J Phy
24 (2000) , 123 – 127.

The Lattice Dynamics of bcc Titanium

Kemal ÇOLAKOĞLU & Yasemin ÇİFTCİ
Gazi University,Faculty of Arts and Sciences,
06500 Ankara-TURKEY

Received 23.06.1999

Abstract

Using in measurements of the phonon frequencies of bcc Titanium, the lattice dynamical calculations are performed on the same phase by using the Third-neighbour Clark-Gazis-Wallis(CGW) model. The theory is used to compute the phonon dispersion curves, the frequency spectra and the lattice spesific heat of the studied phase. The obtained results are compared with the available experimental data.

1. Introduction

As is well known, the transition metals of groups III-VI exhibit stable bcc structure in a certain temperature range at normal pressure. However, upon lowering the temperature, all metals of groups III and IV transform martensitically to hcp(α)[1] structure. For the group-IV metals, a second martensitic phase transition from bcc to hexagonal structure is observed, a generally occuring under pressure of 40 kbar at room temperature [2]. This gradation from weak to very stable bcc transition metals is also reflected in the self-diffusion behaviour [3,4]. To understand the phase systematics of the phase stability of bcc metals, it is of fundemental interest to know their lattice dynamical behaviours.

With measurements of the phonon frequencies of Ti in bcc phase, Sexane et al.[5] very recently, studied the lattice dynamical behavior of bcc Zr and Ti on the basis of the temperature dependent pair potential using a pseudopotential treatment. The present work is the second theoretical and the first Angular Force model application on the lattice dynamics of bcc Ti. In this work, an angular force model (CGW), orginally proposed by Clark- Gazis-Wallis [6] and later improved by Moore and Upadhyaya[7], and Upadhyaya et al[8], is used to reproduce the phonon frequencies of bcc Ti.

2. Theory

2.1. Dynamical Matrix for bcc Structure (third-nearest neighbor)

In the harmonic and adiabatic approximations, the phonon frequencies of cubic systems are determined by solving the usual equation, given by

$$| D(q) - w^2 MI | = 0, \tag{1}$$

where w, M and I have their usual meanings. By following the Moore and Upadhyaya [7], and Upadhyaya et al [8] one can write dynamical matrix elements for ion-ion interactions, appliying the CGW model up to third- nearest neighbour, as follows:

$$\begin{aligned} D_{11} &= \frac{8}{3}(\alpha_1 + 2\acute{\alpha_1})(1 - C_1C_2C_3) + 4\alpha_2 S_1^2 + 4\acute{\alpha_2}(S_2^2 + S_3^2) + \\ &\quad 2(\alpha_3 + \acute{\alpha_3})(2 - C_{21}C_{22} - C_{21}C_{23}) + 4(\acute{\alpha_3} + \alpha_3^N)(1 - C_{22}C_{23}) \\ D_{12} &= \frac{8}{3}(\alpha_1 - \acute{\alpha_1})S_1S_2C_3 + 2(\alpha_3 - \acute{\alpha_3})S_{21}S_{22} \end{aligned} \tag{2}$$

where $S_i = \sin q_i\frac{a}{2}$, $C_i = \cos q_i\frac{a}{2}$, $S_{2i} = \sin q_i a$, $C_{2i} = \cos q_i a$, $i = 1, 2, 3$, and a is the lattice constant. The parameters of this model are given as follows:

$$\begin{aligned} \alpha_1 &= \beta_1 + \frac{16}{3}\gamma_2 + \frac{8}{3}\gamma_4, \\ \alpha_2 &= \beta_2 + \frac{32}{9}\gamma_1 + 4\gamma_6, \\ \alpha_3 &= \beta_3 + \frac{8}{9}\gamma_3 + \gamma_5 + \frac{3}{2}\gamma_7, \\ \acute{\alpha_1} &= \frac{8}{3}\gamma_1 + \frac{4}{3}\gamma_2 + \frac{16}{3}\gamma_3 + \frac{8}{4}\gamma_4, \\ \acute{\alpha_2} &= \frac{4}{3}\gamma_2 - \frac{8}{9}\gamma_1 + 4\gamma_5 + 2\gamma_6, \\ \acute{\alpha_3} &= -\gamma_5 + \frac{\gamma_7}{2}, \\ \alpha_3^N &= -\frac{16}{9}\gamma_3 - \frac{2}{3}\gamma_4 + \gamma_5 + \frac{\gamma_7}{2}, \end{aligned} \tag{3}$$

where $\beta_1, \beta_2, \beta_3$ (central), $\gamma_1, \gamma_2, \gamma_3$ and γ_5 (angular) are the force constants to be determined for this model. By expanding the secular determinant, Eq. 1, in the long-wavelength limits the following relations between elastic constants, C_{11}, C_{12} and C_{44}, and force constants are obtained:

$$aC_{11} = \frac{2}{3}\beta_1 + 2\beta_2 + 4\beta_3 + \frac{16}{3}(2\gamma_1 + \gamma_2 + \gamma_3),$$

$$aC_{12} = \frac{2}{3}\beta_1 + 2\beta_3 - \frac{8}{3}(2\gamma_1 + \gamma_2 + 2\gamma_3), \tag{4}$$
$$aC_{44} = \frac{2}{3}\beta_1 + 2\beta_3 + \frac{8}{9}(2\gamma_1 + 9\gamma_2 + 2\gamma_3 + 9\gamma_5).$$

The bulk modulus of electron gas in CGW model is also given for the bcc structure as

$$K_e = \frac{2}{3}(\alpha_1 + \alpha_2) - \frac{4}{3}(\acute{\alpha_1} + \acute{\alpha_2} + \acute{\alpha_3}). \tag{5}$$

The model parameters (β_1,$\beta_2, \beta_3, \gamma_1$,$\gamma_2, \gamma_3, \gamma_5$)are caculated by using Equations (3), (4), (5) and phonon frequency relations for $\nu_L(100)$, $\nu_L(110)$, $\nu_{T1}(110)$, $\nu_L(111)$. The input data and calculated force constants are given in Table 1.

Table 1. Input Data[1] and Calculated Force Constants for bcc Ti.

Input Data		**Calculated Force Constant**	(dyn/cm)
$(\dot{A})$	3.315	β_1	36532.830
M(a.m.u.)	47.90	β_2	9996.769
$C_{11}(10^{12}dyn/cm^2)$	1.34	β_3	3045.346
$C_{12}(10^{12}dyn/cm^2)$	1.10	γ_1	-1096.769
$C_{44}(10^{12}dyn/cm^2)$	0.36	γ_2	-3143.589
$\nu_L(100)(\xi = 1.0)$	6.30	γ_3	1534.918
$\nu_L(110)(\xi = 0.5)$	6.37	γ_5	735.5291
$\nu_{T1}(110)(\xi = 0.5)$	3.38		
$\nu_L(111)(\xi = 0.5)$	5.07		

The obtained results for the phonon frequencies of bcc Ti in principal symmetry directions are plotted in Figure 1. The obtained force constants are then used to calculate the frequency distribution function $g(\nu)$ as a function of frequency using the algorithm of Glat and Raubenheimer [9], and spesific heat C_v at diffrent temperatures from formula (6) given by [10].

$$C_v = (\frac{3R}{3000})\sum_{\nu} E(\frac{h\nu}{kT})g(\nu), \tag{6}$$

where $g(\nu)$is the frequency distribution function, R the gas constant, and $E(h\nu/kT)$the Einstein function defined by

$$E(x) = \frac{x^2 e^x}{(e^x - 1)^2} \tag{7}$$

here, $x = h\nu/kT$.

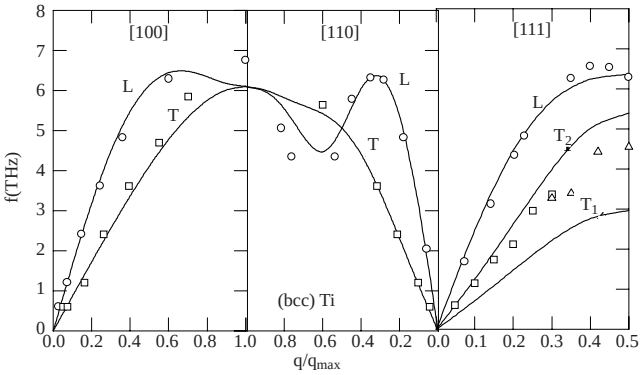

Figure 1. Phonon dispersion curves along the principal symmetry directions of bcc Ti. The solid curves show the present calculations; ○, □ denote the experimental points [1].

3. Results and Discussions

The phonon dispersion curves obtained by using the present model are given in Figure 1. It can be seen that the present model gives satisfactory description of phonon dispersion of the studied metal. The theoretical results given by Sexena et al. [5] exhibit some deviations from experiment, especially, for L(110) and L(111) longitidunal branches. Their two-body potential can be the cause of these deviations. Esentially, the CGW model is a three- body force constant method, and superior to other angular force methods because of the three-body interaction charecter.

The calculated frequency distribution and specific heat curves are given in Figure 2, and Figure 3, respectively, and they show the expected behaviours at low ($\theta \preceq 10/T$)and high temperature values.

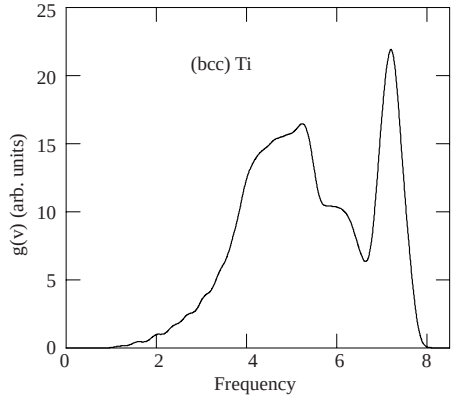

Figure 2. Frequency distribution curves for bcc Ti.

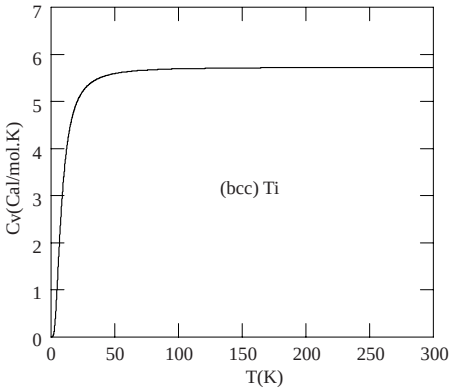

Figure 3. Spesific heat curves for bcc Ti.

It may be concluded that the present model represents, correctly, the actual intereactions responsible for the lattice vibrations in the studied crystal.

References

[1] W. Petry, A.Heiming, J. Trampenau, M.Alba, C. Herzig, H.R. Schober, G. Vogl, *Phys.Rev. B*,**43** (1991) 10933.

[2] S.K. Sikka, Y. K. Vahra, and R.Chidambaram, *Prog. Mater. Sci.* ,**27** (1982) 245.

[3] C. Herzig and U. Kökler, *Mater Sci. Forum*, **15-18** (1988) 301.

[4] W. Petry, A. Heiming, J. Trampenau, G. Vogl, edited by F. J. Kedves and D. L. Beke *Trans. Tech. Publ. Switzerland*, **66-69** (1989) 157.

[5] S.K. Sexana, R.M. Agrawal and R.P.S. Rathore, *Phys. Stat. Sol. b*, **192** (1995) 45.

[6] B.C. Clark, D.C. Gazis and R.F. Wallis,*Phys. Rev. A*, **134**(1964) 1486.

[7] R. A. Moore and J.C. Upadhyaya, *Can. J. Phys.*, **57** (1979) 2053.

[8] J.C. Upadhyaya, S. Lehri, D.K. Sharma, S.C. Upadhyaya, *Phys. Stat. Sol. b*, **159** (1990) 659.

[9] G. Gilat and L.J. Raubenheimer,*Phys. Rev.*, **144**,(1966) 390.

[10] V.K. Thakur, *Phys. Stat. Sol.b*, **135** (1986) 67.