Lattice Dynamical, Elastic, Thermodynamic Properties and Sound Velocities of 3C-SiC

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(Received August 11, 2016; in final form March 29, 2018)

We present a theoretical investigation of lattice dynamical properties, the zone boundary phonons, elastic properties, sound velocities and the Debye characteristic temperature for 3C-SiC using eleven parameter three-body shell model with both the ions polarizable. We compare our calculated results with the experimental and theoretical results.

DOI: [10.12693/APhysPolA.134.478](https://doi.org/10.12693/APhysPolA.134.478)

PACS/topics: silicon carbide, elastic properties, semiconductor, lattice dynamics, phonons

1. Introduction

Silicon carbide in cubic phase (3C-SiC) is a wide band gap semiconductor and has many technological applications in optoelectronic devices and for high-power, high-temperature applications due to its many unique properties such as low density, high strength, high melting point, high hardness large thermal conductivity, high breakdown voltage, and outstanding mechanical and chemical stability.

Recently, the lattice dynamical properties of SiC in zinc-blende (ZB) phase are studied by many researchers using first principles methods [1–4] and phenomenological models [5, 6]. But the exact information about dynamical properties is still missing. Therefore in the present paper, we used eleven parameter three-body shell model with both the ions polarizable and investigated the lattice dynamical properties such as phonon dispersion relations, phonon density of states, variation of the Debye temperature with absolute temperature, zone-boundary phonons, elastic constants, mechanical properties of SiC in ZB phase.

2. Potential model

In three-body shell model proposed by Kushwaha [7], the harmonic potential energy per unit cell for ZB structure compounds can be written as

$$\varphi = \varphi^{SM} + \varphi^{TB}, \quad (1)$$

where φ^{SM} and φ^{TB} are the potential energies of ZB structure compounds in the framework of rigid shell model (RSM) and three-body interaction, respectively.

The secular determinant, for determining the angular frequencies of vibration for the crystals may be obtained by solving the characteristic equation

$$|D_{\alpha\beta}(\mathbf{q}, kk') - \omega^2 \delta_{\alpha\beta} \delta_{kk'}| = 0 \quad (2)$$

for various wave vectors $\mathbf{q}$ in the reciprocal space. The

symbols $k, k' = 1, 2$ represent the type of atoms in the unit cell and $D_{\alpha\beta}(\mathbf{q}, kk')$ are the elements of dynamical matrix.

3. Results and discussion

3.1. Lattice dynamical properties

Our three-body shell model involved 11 parameters as $A, A_1, A_2, \gamma_1, \gamma_2, \gamma_3, \alpha_1, \alpha_2, d_1, d_2$ and Z' , where A, A_1 , and A_2 are two-body short-range parameters between Si–C, Si–Si, and C–C, respectively, γ_1, γ_2 , and γ_3 are three two-body short-range parameters, α_1 and α_2 are electronic polarizabilities, d_1 and d_2 are distortion polarizabilities and Z' — effective charge parameter. The procedure of calculation of force parameters for 3C-SiC is given elsewhere [7]. The input and calculated output parameters for the 3C-SiC is shown in Table I. Using the eleven calculated parameters, we have calculated the phonon dispersion relations for 3C-SiC in three high symmetry directions, as shown in Fig. 1, and these results

TABLE I

The input and output parameters for 3C-SiC

Input parameter		Output parameter	
a	4.40 Å	A	150.28 kdyne/cm
C_{11}	390 Gdyne/cm ²	A_1	8.31 kdyne/cm
C_{12}	142 Gdyne/cm ²	A_2	25.22 kdyne/cm
m_1	26×10^{-24} g	γ_1	4.21 kdyne/cm
m_2	12×10^{-24} g	γ_2	2.89 kdyne/cm
$\omega_{LO}(\Gamma)$	971 1/cm	γ_3	1.71 kdyne/cm
$\omega_{TO}(\Gamma)$	795 1/cm	α_1	0.34×10^{-24} cm ³
$\omega_{LO}(X)$	829 1/cm	α_2	0.61×10^{-24} cm ³
$\omega_{TO}(X)$	760 1/cm	d_1	0.02
ε_0	5.98	d_2	0.05
ε_∞	6.52	Z'	0.81
e	4.8×10^{-10} esu		

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Fig. 1. Phonon dispersion relations 3C-SiC along with the experimental results [2].

TABLE II

Zone-centre and zone-boundary phonons [cm^{-1}] for 3C-SiC. First line — this work, second line experimental [7], third line calculation [8].

Γ_{TO}	Γ_{LO}	X_{TO}	X_{LO}	X_{TA}	X_{LA}	L_{LA}	L_{TA}	L_{TO}	L_{LO}
96	973	763	828	375	637	611	263	764	838
795	972	760	829	372	639	610	261	765	837
783	956	755	829	366	629	610	261	766	838

are in good agreement with the available experimental results [2]. We have also calculated the zone-centre and zone boundary phonons for 3C-SiC and these are listed in Table II along with the previous experimental and theoretical data [3, 8].

Fig. 2. Phonon density of states of 3C-SiC.

Fig. 3. Θ_D versus T curve for 3C-SiC.

Phonon density of states has been calculated by the Blackman sampling technique [9]. For the calculation of phonon density of states and the Debye characteristics temperature we have used the method given in the literature [10]. The calculated phonon density of states and the variation of the Debye characteristics temperature with the absolute temperature are shown in Figs. 2 and 3, respectively.

3.2. Elastic and related properties

For cubic systems, we have three elastic constants C_{11} , C_{12} , and C_{44} and these are calculated by the method given in the literature [11]. The calculated elastic constants and related properties such as bulk modulus, compressibility, the Young modulus, shear modulus, the Poisson ratio and anisotropy factor are listed in Table III along with the previous experimental and theoretical results [12–38] available in the literature.

TABLE III

Calculated elastic constants C_{11} , C_{12} , and C_{44} (GPa), bulk modulus B (GPa), compressibility coefficient K (GPa^{-1}), shear modulus G (GPa), the Young modulus Y (GPa), the Poisson ratio σ , anisotropy factor A for 3C-SiC. First line — this work, lower lines — others.

C_{11}	C_{12}	C_{44}	B	K	G	Y	A	σ
38.7	15.2	26	23.0	0.044	18.9	44.5	2.21	0.647
39.0 ^a	14.2 ^a	25.6 ^a	22.7 ^k	0.024 ^e	19.2 ^m	44.8 ^m		0.267 ^a
36.3 ^b	15.4 ^b	14.9 ^b	22.4 ^l	1.01 ^o	16.5 ^e	41.2 ^e		0.168 ^m
			22.5 ^m	1.12 ^p	21.9 ^s	49.6 ^t		0.249 ^e
42.0 ^c	12.6 ^c	28.7 ^c	22.3 ^c		16.9 ^d	40.1 ^d		0.146 ^t
35.2 ^d	14.0 ^d	23.3 ^d	21.1 ^d		12.4 ⁱ	56.7 ^q		0.201 ^d
37.1 ^e	22.3 ^e	27.9 ^e	27.3 ^f		14.1 ^b	55.0 ^q		0.268 ⁱ
44.9 ^f	14.6 ^f	25.6 ^f	24.9 ⁿ			31.4 ⁱ		1.0 ^p
43.6 ^g	12.0 ^g	25.5 ^g	22.5 ^o			35.2 ^b		0.259 ^b
39.0 ^h	14.4 ^h	17.9 ^h	21.2 ^p					
39.0 ⁱ	14.3 ⁱ	19.1 ⁱ	22.5 ^{q,h,i,r,b}					
37.1 ^b	16.9 ^b	17.6 ^b	22.7 ^j					
41.5 ^j	13.19 ^j	26.5 ^j	20.0 ^s					

^a [11], ^b [12], ^c [13], ^d [14], ^e [15], ^f [16, 17], ^g [18], ^h [19], ⁱ [20, 21],
^j [22], ^k [23], ^l [24], ^m [25], ⁿ [26], ^o [27], ^q [28, 29], ^p [30–33],
^r [34, 35], ^s [36], ^t [37]

TABLE IV

Elastic wave velocities [km/s] in various directions and the Debye temperature [K] for 3C-SiC. First line — this work.

$v_L^{[100]}$	$v_T^{[100]}$	$v_l^{[110]}$	$v_t^{[110]}$	$v_{t\perp}^{[110]}$	$v_{v_l'}^{[111]}$	$v_{v_t'}^{[111]}$	V_L	V_T	V_m	Θ_D
3.47	2.85	4.06	2.85	1.91	4.24	2.27	12.21	7.69	3.32	691
					calc.	[32]	12.40	7.17	16.88	612
					calc.	[15]	12.44	7.82	1.82	709
					calc.	[39]	12.18	7.70		

The calculated sound velocities along high symmetry directions and the Debye temperature for 3C-SiC are given in Table IV along with the previously calculated results [32, 15, 39].

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