J. Phys. &Chem. Res. 3, Issue 1, June (2024) 26–33

Journal of Physical & Chemical Research

Journal homepage:https://ojs.univ-bba.dz

Thermodynamic Grüneisen parameter and thermal expansion coefficient of β-SiC

Nadhira Bioud [1, 2], **Nadjima Benkara-Mohammed** [1] **and Nadjet Benchiheub**[3,*]

[1]*Faculty of Sciences and Technology, University Mohamed El Bachir EL IBRAHIMI of Bordj Bou Arreridj, 34000, Bordj Bou Arreridj, Algeria.*
[2] *Laboratoire d'Optoélectronique et Composants, Faculté des sciences, Université FERHAT ABBAS de Sétif1, 19000, Sétif, Algérie.*
[3]*Laboratory of Materials Physics, Radiation and Nanostructures (LPMRN), Faculty of Sciences and Technology, University Mohamed El Bachir EL IBRAHIMI of Bordj Bou Arreridj, 34000, Bordj Bou Arreridj, Algeria.*

* *Corresponding author: E-mail address: nadjat.benchiheub@univ-bba.dz.*

Article history
Received November 13, 2024
Accepted for publication December 9, 2024

Abstract

The purpose of this study is to calculate the thermodynamic Grüneisen parameter γ as well as the volumetric thermal expansion coefficient α of the cubic zinc-blende silicon carbide (β-SiC) compound by using the quasi-harmonic Debye model. The details of the calculation method adopted here are presented elsewhere (*Silicon*, 14(17), (2022) 6299 – 6309). Our findings relative to both the Grüneisen parameter and the volumetric thermal expansion coefficient refer to a decrease with increasing pressure in the range from 0 to 60 GPa and an increase with increasing temperature in the range from 0 to 1500 K, respectively. As the Grüneisen parameter is associated with the phonon frequency distribution, it reduces as the pressure increases and increases as the temperature rises. At zero pressure and T = 300 K, our predicted value of the Grüneisen parameter is around 1.82, while at p = 0 and T = 1500 K, it reaches the value of 1.95.

Keywords: Silicon-carbide; Thermal expansion; High pressure; Quasi-harmonic Debye model; HighTemperature.

1. Introduction

Based upon the results of some previous studies carried out on IV-IV group carbides such as GeC and SnC compounds that identify potential technological applications of these materials in extreme conditions [1], we present an investigation of the Silicon carbide (SiC) semiconducting material. Actually, this material of interest is being investigated as a promising material for the third generation of semiconductors after the first and second-generation materials. It has been used in lighting and power electronics [1].

Due to its excellent physical and electronic properties, the Silicon Carbide (SiC) compound has attracted the attention of numerous researchers [2]. Note that SiC has high thermal conductivity, excellent mechanical strength, wide band gap, and low thermal expansion, which allow for the design of an innovative semiconducting material compared to silicon [2].

In their work, Lebga *et al.* [3] studied the second and third-order elastic constants of β-SiC. Meanwhile using density functional theory (DFT) within the local density approximation (LDA) and the pseudopotential plane-wave (PP-PW) method. Daoud *et al.* [4] investigated the structural parameters and the structural phase transition of the cubic silicon carbide (3C-SiC) using first-principles calculations. They found that the cubic zinc-blende phase of SiC transforms to the rock-salt phase at a pressure of around 70 GPa. They also studied the thermodynamic properties of -SiC using the quasi-harmonic Debye model.

To study the effects of temperature and grain size on the mechanical properties of nanocrystalline SiC, Kuryliuk *et al.* [5] employed molecular dynamics (MD) simulations. They estimated Young's modulus E from the slope of stress-strain $\sigma(\varepsilon)$ curves. They found that temperature significantly affects Young's modulus, which is attributed to the large volume fraction of grain boundaries in the samples.

In the same context, Abdul-Hafihd and Aïssa [6] developed thermodynamical models, aiming to predict the dependence with pressure and the temperature of the bulk modulus for spherical SiC nanoparticles (NPs).

To extend the understanding of SiC properties, we propose to calculate the thermodynamic Grüneisen parameter and the volumetric thermal expansion coefficient of β-SiC using the quasi-harmonic Debye model. The details of the quasi-harmonic Debye model and the method of calculations adopted in the present investigation are presented elsewhere [4].

2. Method of calculation

Knowing that the experimental processes used in the production of materials significantly influence their behavior. Similarly, in simulations, the calculation method can play a predominant role. We used the quasi-harmonic Debye model approximation to investigate the dependence of the thermodynamic Grüneisen parameter and the volumetric thermal expansion coefficient of the β-SiC on the pressure in the range from 0 to 60 GPa and temperature in the range from 0 to 1500 K. Our calculations were implemented using the GIBBS code [7, 8], which requires total energy - volume (*E*-*V*) as input data. For more details on the *E*-*V* input data and the method of calculation adopted in the present work, please consult Ref. [4].

3. **Results and discussion**

3.1. Thermodynamic Grüneisen parameter

In the quasi-harmonic Debye model approximation, the thermodynamic Grüneisen parameter γ, the volume V, and the Debye temperature θ_D are related by the following formula [7, 9]:

$$\gamma = - \partial \ln\theta_D(V)/\partial \ln V \tag{1}$$

Both temperature and pressure are basic thermodynamic variables, which can transform matter from one state to another. Usually, the Grüneisen parameter γ decreases as the pressure increases [10, 11]. Figure 1 shows the dependence of the Grüneisen parameter γ for β-SiC as a function of pressure at four different temperatures (0, 300, 1000, and 1500 K).

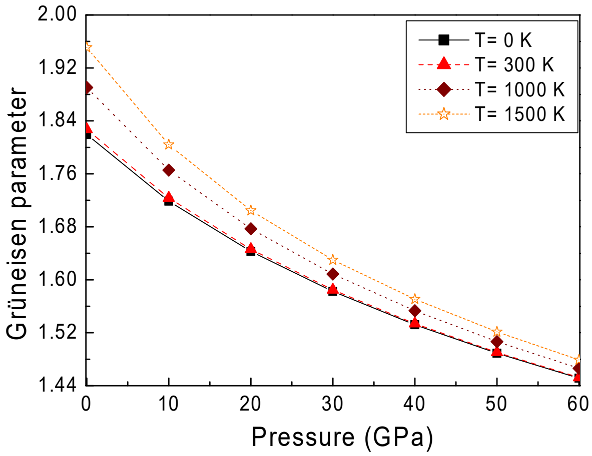

Figure 1. Thermodynamic Grüneisen parameter γ *vs* pressure for β-SiC at various temperatures (0, 300, 1000, and 1500 K).

From Figure 1, we can observe that γ decreases monotonically with increasing pressure. The same behavior of the Grüneisen parameter γ under pressure was also observed in several materials, such as in cubic rock-salt aluminum nitride (AlN) [12], in calcium chalcogenides CaX (X = S, Se, Te) compounds [13], in CdSe, $Cd_{0.75}Cr_{0.25}Se$, ZnS and $Zn_{0.75}Cr_{0.25}S$ materials [14] in CaO compound [15] as well as in Cu_2ZnSnS_4 semiconductor [16]. At zero-pressure and $T = 0$ K, our value of γ for β-SiC is around 1.82, while at zero- pressure and $T = 1500$ K, it reaches a value of 1.95. At zero-pressure and $T = 0$ K, our value (1.82) of γ for β-SiC is lower than the calculated value ~ 2.15 reported for the ordered $Ge_{0.5}Sn_{0.5}$ cubic alloy in the zinc-blende phase [9].

At temperatures of 0, 300, 1000 and 1500 K, the fits of our data regarding the Grüneisen parameter γ for β-SiC obey the following quadratic expressions, respectively:

$$\gamma = 1.80 - 8.08 \times 10^{-3} p + 3.5 \times 10^{-5} p^2 \tag{2a}$$

$$\gamma = 1.81 - 8.25 \times 10^{-3} p + 3.6 \times 10^{-5} p^2 \tag{2b}$$

$$\gamma = 1.87 - 9.47 \times 10^{-3} p + 4.38 \times 10^{-5} p^2 \tag{2c}$$

$$\gamma = 1.92 - 1.07 \times 10^{-2} p + 5.15 \times 10^{-5} p^2 \tag{2d}$$

where the pressure is expressed in GPa.

Figure 2 shows the dependence of the Grüneisen parameter γ as a function of temperature at different pressures. From Figure 2, we can observe that γ increases slowly with increasing temperature. At a pressure of 60 GPa, γ is almost unchangeable with the temperature rise. As the Grüneisen parameter is associated with the phonon frequency distribution, it reduces as the pressure increases and enhances as the temperature increases. The same behavior for γ under temperature was also observed in cubic zinc-blende copper iodide (CuI) material [17].

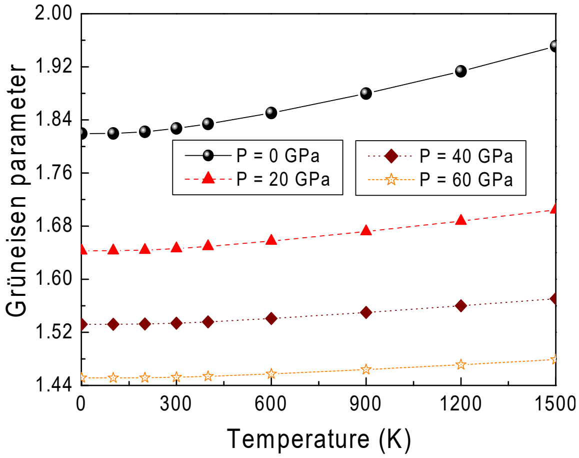

Figure 2. Thermodynamic Grüneisen parameter γ *vs* temperature for *β*-SiC at various pressures (0, 20, 40, and 60 GPa).

By fitting the Grüneisen parameter γ as a function of temperature T (expressed in K), the following quadratic relationships can be obtained at 0, 20, 40, and 60 GPa, respectively:

$$\gamma = 1.82 + 3.36 \times 10^{-5}T + 3.83 \times 10^{-8}T^2 \tag{3a}$$

$$\gamma = 1.64 + 1.69 \times 10^{-5}T + 1.75 \times 10^{-8}T^2 \tag{3b}$$

$$\gamma = 1.53 + 0.96 \times 10^{-5}T + 1.17 \times 10^{-8}T^2 \tag{3c}$$

$$\gamma = 1.45 + 0.59 \times 10^{-5}T + 0.90 \times 10^{-8}T^2 \tag{3d}$$

3.2. Volumetric thermal expansion coefficient

The coefficient of thermal expansion (CTE) of a material defines how its length changes in response to a variation in temperature [2]. Matching the thermal expansion coefficients of components enhances the robustness and lifetime of devices in electrical and mechanical systems by reducing the chance of internal residual stresses forming due to temperature cycling [2]. In the quasi-harmonic Debye model, the volumetric thermal expansion coefficient α is given as follows [7, 9]:

$$\alpha = \frac{\gamma C_V}{B_T V} \tag{4}$$

where γ is the Grüneisen parameter, C_V is the vibrational heat capacity, B_T is the isothermal bulk modulus and V is the volume.
Figure 3 shows the dependence of the volumetric thermal expansion coefficient α for β-SiC as a function of pressure at different temperatures (300, 500, 1000, and 1500 K). We can observe that the volumetric thermal expansion coefficient α decreases with increasing pressure.

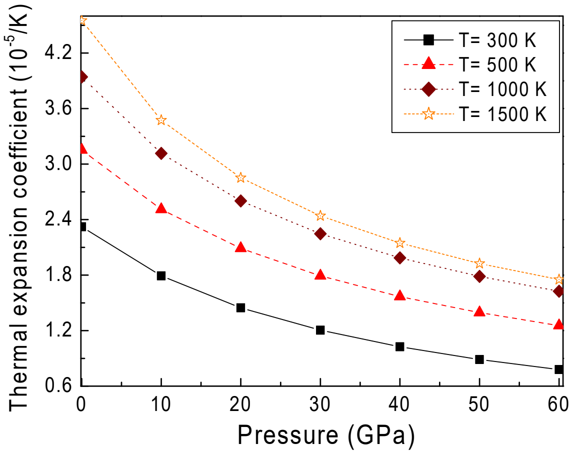

Figure 3. Volumetric thermal expansion coefficient α *vs* pressure for β-SiC at various temperatures (300, 500, 1000, and 1500 K).

At temperatures of 300, 500, 1000, and 1500 K, the fits of our data on the volumetric thermal expansion coefficient α (expressed in 10^{-5}/K) for β-SiC obey the following quadratic expressions, respectively:

$$\alpha = 2.20 - 3.71 \times 10^{-2} p + 2.1 \times 10^{-4} p^2 \quad (5a)$$

$$\alpha = 3.00 - 4.52 \times 10^{-2} p + 2.5 \times 10^{-4} p^2 \quad (5b)$$

$$\alpha = 3.74 - 5.55 \times 10^{-2} p + 3.1 \times 10^{-4} p^2 \quad (5c)$$

$$\alpha = 4.26 - 6.77 \times 10^{-2} p + 4.0 \times 10^{-4} p^2 \quad (5d)$$

where the pressure is expressed in GPa.

Unfortunately, our predicted value of the volumetric thermal expansion coefficient α of β-SiC at ambient conditions appears much higher than the experimental linear thermal expansion coefficient (2.2×10^{-6}/°C) reported by Sultan *et al.* [2]. Figure 4 shows the dependence of α for β-SiC as a function of temperature at different pressures (0, 20, 40, and 60 GPa). From this figure, we can observe that α increases with increasing temperature. It is shown that the thermal expansion coefficient increases abruptly with the rise in temperature up to ~ 600 K. When T > 600 K, it increases slowly with further temperature increase and becomes almost linear at high temperatures.

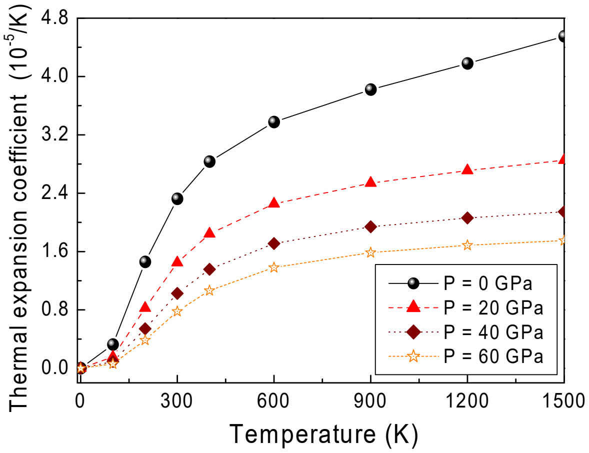

Figure 4. Volumetric thermal expansion coefficient α vs temperature T for β-SiC at various pressures (0, 20, 40 and, 60 GPa).

We note that the same behavior for α under temperature was also observed in several materials, such as in the ordered $Ge_{0.5}Sn_{0.5}$ cubic alloy in the zinc-blende phase [9], in cubic rock-salt AlN compound [12], in Cu_2ZnSnS_4 quaternary semiconductor [16], in zinc-blende copper iodide material [17], in both boron phosphide (BP) and boron arsenide (BAs) semiconductors

[18], in cubic rock-salt strontium-based chalcogenides SrX (X = O, S, Se and Te) materials [19], and in the post-perovskite $MgSiO_3$ material [20].

4. Conclusion

The quasi-harmonic Debye approach has been applied to obtain the pressure and temperature dependence of the Grüneisen parameter γ and the volumetric thermal expansion coefficient of β-SiC. The results obtained are analyzed and interpreted. We found that both the Grüneisen parameter γ and the volumetric thermal expansion coefficient α of β-SiC decrease with increasing pressure in the range from 0 to 60 GPa, and increase with rising temperature in the range from 0 to 1500 K, respectively. We note that the same behaviors for γ and α under pressure and temperature were also observed in several materials.

References

[1] H. Muñoz, J. E. Antonio, J. M. Cervantes, J. L. Rosas-Huerta, E. Carvajal, R. Escamilla, First-principles study of the effect of pressure on the physical properties of PbC, Mater. Res. Express, Vol.10, (2023) 055601. https://doi.org/10.1088/2053-1591/acd323

[2] N. M. Sultan, T. M. B. Albarody, H. K. M. Al-Jothery, M. A. Abdullah, H. G. Mohammed, K. O. Obodo, Thermal expansion of 3C-SiC obtained from in-Situ X-ray diffraction at high temperature and first-principal calculations, Materials, Vol.15, (2022) 6229. https://doi.org/10.3390/ma15186229

[3] N. Lebga, K. Bouamama, P. Djemia, S. Mourad Chérif, Theoretical study of second and third order elastic constants of β-SiC, J. Phys. & Chem. Res., Vol.1, No. 2, (2022) 16–24. https://doi.org/10.58452/jpcr.v1i2.23

[4] S. Daoud, N. Bouarissa, H. Rekab-Djabri, P. K. Saini, Structural and thermophysical properties of 3C-SiC: High-temperature and high-pressure effect, Silicon, Vol.14, No. 17, (2022) 6299 – 6309. https://doi.org/10.1007/s12633-021-01387-8

[5] A.N. Kuryliuk, K.V. Maliutiak, V.V. Kuryliuk, Molecular dynamics modeling of mechanical properties of nanocrystalline SiC, J. Nano-Electron. Phys., Vol.11, No. 2, (2019) 02001 (5pp). https://doi.org/10.21272/jnep.11(2).02001

[6] Esam H. Abdul-Hafih, Brahim Aïssa, Development of a thermodynamical approach for the prediction of the bulk modulus of spherical cubic silicon carbide ($\beta-$SiC) nanosolids, Results in Engineering 17 (2023) 100836. https://doi.org/10.1016/j.rineng.2022.100836

[7] M. A. Blanco, E. Francisco, V. Luaña, GIBBS: Isothermal-isobaric thermodynamics of solids from energy curves using a quasi-harmonic Debye model, Comput. Phys. Commun., Vol.158, (2004) 57–72. https://doi.org/10.1016/j.comphy.2003.12.001

[8] A. Otero-de-la-Roza, V. Luaña, GIBBS 2: A new version of the quasiharmonic model code. II. Models for solid-state thermodynamics,

features, and implementation, Comput. Phys. Commun., Vol.182, (2011) 2232–2248. https://doi.org/10.1016/j.cpc.2011.05.009

[9] X.D. Zhang, C.H. Ying, S.Y. Quan, Z.J. Li, Ab initio study of the structural, phonon, elastic and thermodynamic properties of the ordered $Ge_{0.5}Sn_{0.5}$ cubic alloy under high pressure, Comput. Mater. Sci., Vol. 58, (2012) 12–16. https://doi.org/10.1016/j.commatsci.2012.02.004

[10] N. Benkara-Mohammed, N. Bioud, N. Benchiheub, Hydrostatic pressure response of semiconducting GaSb applying a semi-empirical approach, Comput. Condens. Matter, Vol.39, No. 2, (2024) e00895. https://doi.org/10.1016/j.cocom.2024.e00895

[11] N. Bioud, N. Benchiheub, Mechanical and thermal behavior of semiconducting cadmium oxide at high-pressure, Annals of West University of Timisoara-Physics, Vol. 66, (2024) 142–156. https://doi.org/10.2478/awutp-2024-0009

[12] N. Lebga, S. Daoud, X-W Sun, N. Bioud, A. Latreche, Mechanical and thermophysical properties of cubic rock-salt AlN under high pressure, J. Electron Mater., Vol.47, (2018) 3430–3439. https://doi.org/10.1007/s11664-018-6169-x

[13] F. Okba, R. Mezouar, Some physical parameters of calcium chalcogenides at high pressures: Semi-empirical approach, J. Nano-Electron. Phys., Vol.14, No4, (2022) 04004 (4pp). https://doi.org/10.21272/jnep.14(4).04004

[14] S. Amari, S. Daoud, H. Rekab-Djabri, Structural, thermodynamic and magneto-electronic properties of $Cd_{0.75}Cr_{0.25}Se$ and $Zn_{0.75}Cr_{0.25}S$: An ab-initio study, Acta Phys. Pol. A, Vol. 143, No. 1, (2023) 36–46. https://doi.org/10.12693/APhysPolA.143.36

[15] N. Bioud, N. Benchiheub, Pressure effect on some physical properties of calcium oxide material, Chem. Phys. Impact, 7 (2023) 100342 (5 pp). https://doi.org/10.1016/j.chphi.2023.100342

[16] S. H. Fan, H. J. Hou, H. L. Guo, DFT study of elastic and thermodynamic properties of solar material Cu_2ZnSnS_4, Journal of Ovonic Research, Vol. 20, No. 5 (2024) 601–615. https://doi.org/10.15251/JOR.2024.205.601

[17] N. Bioud, X-W. Sun, S. Daoud, T. Song, R. Khenata, S. Bin Omran, High-temperature and high-pressure physical properties of CuI with zinc-blende phase by a systematic *ab initio* investigation, Optik, Vol.155, No. 2, (2018) 17 – 25. https://doi.org/10.1016/j.ijleo.2017.11.006

[18] Y. Megdoud, R. Mahdjoubi, M. Amrani, H. Bendjeddou, S. Ghemid, H. Meradji, R. Khenata, Phase stability and physical properties of BAs and BP compounds: an ab-initio study, Comput. Condens. Matter, Vol. 22, (2020) e00434. https://doi.org/10.1016/j.cocom.2019.e00434

[19] D. Varshney, S. Jain, S. Shriya, R. Khenata, High-pressure and temperature-induced structural, elastic, and thermodynamical properties of strontium chalcogenides, J. Theor. Appl. Phys., Vol. 10, (2016) 163–193. https://doi.org/10.1007/s40094-016-0214-z

[20] Z-J. Liu, X-W. Sun, C-R. Zhang, L-N. Tian, Y. Guo, Thermodynamical properties $MgSiO_3$ post-perovskite, Mod. Phys. Lett. B, Vol. 24, No. 3 (2010) 315–324. https://doi.org/10.1142/S0217984910022391