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Mechanical anisotropy and Debye temperature in c-BN material

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Abstract

2 dimensional dependence of mechanical moduli in cubic zincblende boron nitride (c-BN) has been studied using the experimental Brillouin scattering elastic constants C_{ij} (C_{11} = 820 GPa, C_{12} = 190 GPa and C_{44} = 480 GPa) of the litterature (M. Grimsditch, E. S**.** Zouboulis, **A.** Polian, J. Appl. Phys. 76 (1994) 832). The linear compressibility, shear modulus, Young's modulus and Poisson's ratio have been schematized in graphical representations. The maximum value of the shear modulus, G_{max} is 480 GPa, while its minimum value G_{min} is 315 GPa, which gives G_{max}/ G_{min} = 1.524, those of the Young's modulus, E_{max} is 1028.6 GPa and E_{min} is 748.5 GPa, which gives a ratio E_{max}/E_{min} = 1.374; while for the Poisson's ratio υ, the maximum value υ_{max} is 0.236 and the minimum value υ_{min} is − 0.02, which gives an indefinite value (∞) for $\upsilon_{max}/\upsilon_{min}$.

Furthermore, we predict the Debye temperature Θ_D of c-BN compound, it is 1930.5 K from Siethoff's formula and 2057.2 K from Blackman's expression, respectively.

Keywords: Boron nitride, Mechanical moduli, mechanical Anisotropy, Elastic constants, Debye temperature.

1. Introduction

Built from two light atoms in the periodic table, boron nitride (BN) is one of the most fascinating materials. Boron nitride has many extraordinary properties including high thermal stability, low friction coefficient, high mechanical rigidity, low dielectric constant and high chemical stability [1]. All these extraordinary properties make BN stand out from an inorganic insulator with wide applications unlocked, ranged from biomedical, optoelectronics, spintronics, to aerospace sectors [1].
From a theoretical point of view, several works have been devoted to investigate different physical properties of boron nitride [2-6].
Using first-principles calculations based on density functional theory (DFT) method, Fan and co-authors [2] have investigated the structural, elastic, electronic properties and elastic anisotropy of Pbca- boron nitride (Pbca-BN, space group: Pbca). It is found that Pbca-BN is mechanically stable and it is an insulator with wide band gap of ~5.4 eV [2].
Using first-principles molecular dynamics simulation (MDS), Nico de Koker [4] has evaluated the thermodynamics of zincblende solid and liquid boron nitride at extreme temperatures and pressures, while Çetin and Durandurdu [6] have studied the structural and mechanical properties as well as the electronic structure of Boron-rich amorphous boron nitride (B_xN_{1-x}, $0.55 \leq x \leq 0.95$).
In the present work, the directional dependence of the mechanical moduli for c-BN compound has been studied. The elastic constants used here are taken from the litterature (J. Appl. Phys. 76 (1994) 832).

2. Theory, results and discussion

Using the experimental Brillouin scattering elastic constants C_{ij} (C_{11} = 820 GPa, C_{12} = 190 GPa and C_{44} = 480 GPa) of the litterature [7], the expression describing the directional dependence of the elastic moduli of crystals [8] and the procedure presented by Gaillac *et al.* [9], the values gained for the Young modulus E (in GPa), the linear compressibility β (in TPa^{-1}), the shear modulus G (in GPa), and the Poisson's ratio υ as a function of the direction for c-BN are illustrated in 2 dimensions (2D) in Figure 1 (A), (B), (C) and (D), respectively.
The dependence of Young's modulus *E* with the direction could be determined using the following equation [8, 10]

$$E^{-1} = s_{11} - \beta_1 (\alpha^2\beta^2 + \alpha^2\gamma^2 + \beta^2\gamma^2) \quad (1)$$

where α, β, and γ are the direction cosines of the tensile stress direction, $\beta_1 = (2s_{11} - 2s_{12} - s_{44})$ and s_{11} s_{22}, and s_{44} are the elastic compliance constants, respectively.

The maximum and minima values E_{max} and E_{min} are depend to the value of β_1. If $\beta_1 > 0$, the maximum and minima values of E are expressed as $E_{max} = 3/(s_{11} + 2s_{12} + s_{44})$ and $E_{min} = 1/s_{11}$, respectively [8].
For c-BN compound, $\beta_1 = 0.11 \times 10^{-2}$ GPa$^{-1} > 0$, the values E_{max} and E_{min} are equal to 1028.6 GPa along the [111] direction for {110} planes, and 748.5 GPa along [001] direction for {100} planes, respectively. The result of E_{max}/E_{min} ratio obtained in this work is around 1.374.

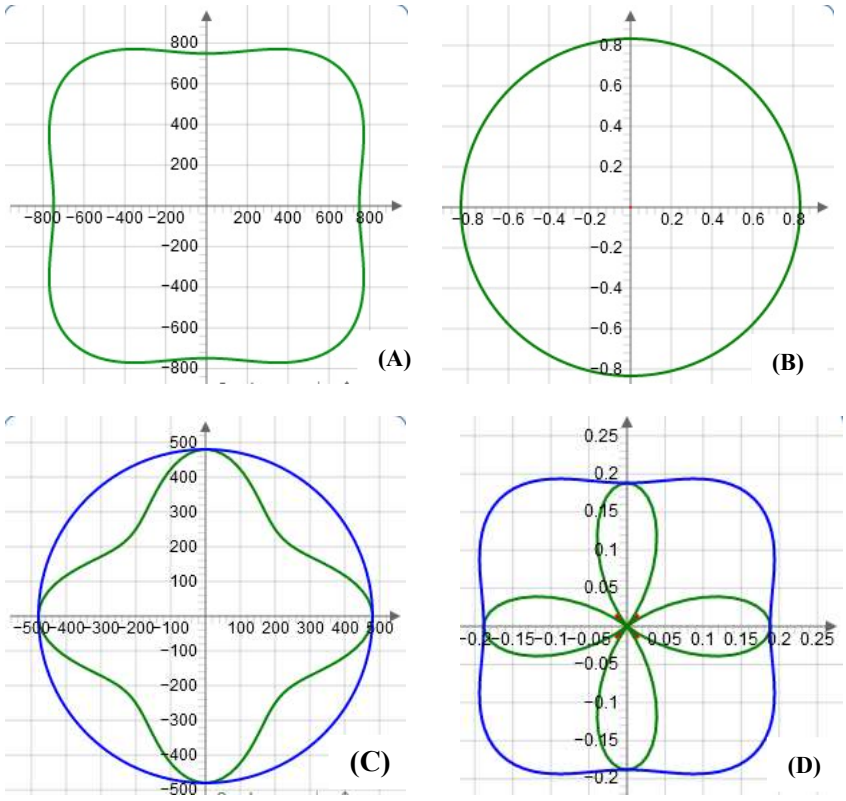

Fig. 1. XY, XZ and YZ planes dependence of Young modulus E (in GPa) (A), linear compressibility β (in TPa^{-1}) (B), shear modulus G (in GPa) (C), and Poisson's ratio υ (D) in c-BN compound.

The maximum value of the shear modulus G, G_{max} is 480 GPa, while its minimum value G_{min} is 315 GPa, which gives $G_{max}/ G_{min} = 1.524$, those of the linear compressibility β are $\beta_{max} = \beta_{min} = \sim 0.833$ TPa^{-1}; while for the Poisson's ratio υ, the maximum value υ_{max} is 0.236 and the minimum value υ_{min} is − 0.02, which gives an indefinite value (∞) for $\upsilon_{max}/\upsilon_{min}$.
Furthermore, we try to predict the Debye temperature Θ_D of c-BN. An expression related the Debye temperature Θ_D to the elastic constants of cubic crystal has been established by Blackman [11], it is given as follows

[11]:

$$\theta_D^3 = \frac{3.15}{8\pi}\left(\frac{h}{k_B}\right)^3\left(\frac{n}{\rho^{3/2}v_a}\right)(C_{11}-C_{12})^{1/2}(C_{11}-C_{12}+2C_{44})^{1/2}(C_{44})^{1/2} \quad (2)$$

Where: k_B is the Boltzmann constant, h is the Planck's constant, n is the number of atoms in unit cell of volume v_a and ρ is the crystal density.
Using the experimental lattice parameter: a = 3.616 Å [12], the calculated values of θ_D for c-BN was found at around 2057.2 K.
The Debye temperature Θ_D is given also as function of the elastic constant C_{ij} by the following formula [13]:

$$\theta_D = C_S s^{-1/6}\left(aGc/M\right)^{1/2} \quad (3)$$

Here a is the lattice parameter, M is the atomic weight (for compounds it is the weighted arithmetical average of the masses of the species), Cs is constant ($Cs = 26.05 \pm 0.81$ K $(m.kg.N^{-1})^{1/2}$, valuable only for crystals with cubic structures), and s is the number of atoms in the unit cell. The elastic constants enter in Eq. (3) via the elastic modulus G, which may be written as follows [13] :

$$Gc = \left[C_{44}\left[C_{44}\left(C_{11}-C_{12}\right)/2\right]^{1/2}\left(C_{11}-C_{12}+C_{44}\right)/3\right]^{1/3} \quad (4)$$

Using the experimental lattice parameter: a = 3.616 Å [12], the value 1930.5 K of the Debye temperature θ_D predicted for c-BN compound from Siethoff's formula [13] is lower than the value (2057.2 K) obtained from Blackman's expression [11], and it is very larger than the theoretical one (1707.56 K) reported by Daoud *et al.* [3].

4. Conclusion

The 2 dimensional dependence of the linear compressibility, Young's modulus, shear modulus, and Poisson's ratio in c-BN compound has been schematized in graphical representations. The maximum and minimum values are, respectively: 480 and 315 GPa for the shear modulus, 1028.6 and 748.5 GPa for the Young's modulus, and 0.236 and −0.02 for the Poisson's ratio υ. The linear compressibility β is ~ 0.833 TPa^{-1}.
Furthermore, we predict the Debye temperature Θ_D of c-BN compound, it is 2057.2 K from Blackman's expression and 1930.5 K from Siethoff's formula, respectively.

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