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First Principle Study of Phonon in BE_2C

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Abstract

The phonon properties of Be_2C of antifluorite structure was computed with ab initio Density Functional Theory calculations using the generalized gradient approximation (GGA). The structure is used as a UV resistive and hard material. The obtained phonon dispersion indicates antifluorite Be2C are dynamically stable and the obtained phonon DOS indicates high oscillations in the higher frequency ranges.

Keywords: *Phonon, Phonon dispersion, Primitive Structure, Conventional Structure, BE_2C,*

Introduction

Be_2C belongs to Group II-IV element antifluorite structure similar to diamond. It is transparent crystalline solid and very hard compound like diamond (Tzeng et al., 1998). It is a refracting material and have large elastic constants (Corkill & Cohen, 1993). It has high resistance to radiation damage and may be used in fission reactor components as a blanket material in fusion reactor (Lee et al., 1995).

The phonon dispersion is obtained from diagonalizing the dynamical matrix containing force constants between any two atoms in a system of interest. The phonon dispersion consists of acoustic phonon mode and optical phonon mode (Varshney et al., 2015). The acoustic phonon is a coherent movement of vibration (in-phase), which means one atom and neighbour atom have vibrate same direction, and the optical phonon is out-of-phase vibration, vice versa. The acoustic phonon has a relatively low frequency, and move to the same phase in the unit cell. It has one longitudinal acoustic mode (LA), having large phonon group velocity, and two transverse acoustic modes (TA) (Maurya et al., 2019). Therefore, acoustic phonons have a great influence on thermal conductivity characteristic which is important to have a large phonon group velocity and a long phonon relaxation time. The optical phonon has high frequency than acoustic phonon and has opposite vibration direction of one atom and neighbour atom. Thus, it has small phonon group velocity and broad energy range than acoustic phonon modes. Especially, it interacts with photon. The out-of-plane vibration cause the dipole moment. Therefore, IR active and Raman active properties of the structure occur due to optical phonon. In this work, phonon calculations are performed by DFPT method for the structure Be2C. Be2C is very common and many properties has been investigated for the compound (Mallett et al., 1954).

Computational Details

The first principle calculations were carried out with DFT package Quantum Espresso (version 7.0) along with pseudopotential plane-wave method. The PBE-PAW pseudopotentials (Singh & Nordstrom, 2006) were used with an energy cutoff of 50 Ry and k-point mesh 8 x 8 x 8 is employed for DFT calculations (Sholl & Steckel, 2011) of optimized structure with total energy converging within 10^{-4} a.u. PBE exchange correlation functional of GGA (Perdew et al., 1996) is used in all calculations.

The phonon calculations were performed through Quantum Espresso (version 7.0) using DFTP method. A 12 x 12 x 12 k-point grid was used for sampling the irreducible segment of the Brillouin zone for phonon calculations. In order to obtain full phonon spectrum, we evaluated 8 dynamical matrices on a 4 x 4 x 4 grid in q space for the structure. These matrices were then Fourier-interpolated to obtain the phonon dispersion curves and DOS.

Results

The Be_2C have a face-centered cubic crystal structure with space group Fm-3m (225) (Ruschewitz, 2003). The occupied Wyckoff positions for Be and C atoms are 8c (0.25, 0.25, 0.25), (0.75, 5 0.75, 0.75) and 4a (0, 0, 0), respectively. The figure 1 shows the crystal structure of the compound Be_2C (Yan et al., 2011).

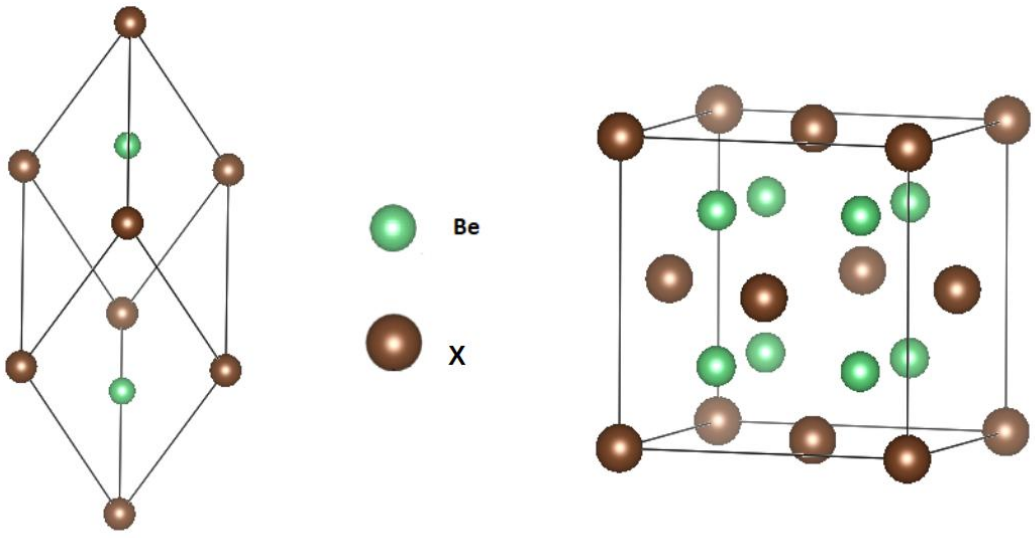

Fig 1: (a) Primitive Structure, (b) Conventional Structure [X = C]

The optimized lattice parameter for the structure is shown in the Table 1 below with available theoretical and experimental value for comparison.

Work	**Method**	**Values**

This Work	GGA	4.327 A
Paliwal et al., 2013	GGA	4.335 A
Yan et al., 2011	GGA	4.33 A
Experimental	-	4.330 A

The primitive cell of Be_2C contained three atoms (Coobs & Koshuba, 1952). The corresponding number of vibrational modes is 9 of which 3 are acoustic branches and the remaining 6 are optical ones. The acoustic modes frequencies converge at high symmetry Gamma point. The phonon frequencies are positive for Be_2C which confirms its dynamical stability (Fowler & Tole, 1989). The phonon dispersion and DOS along majority symmetry directions of the structure is shown in figure 2.

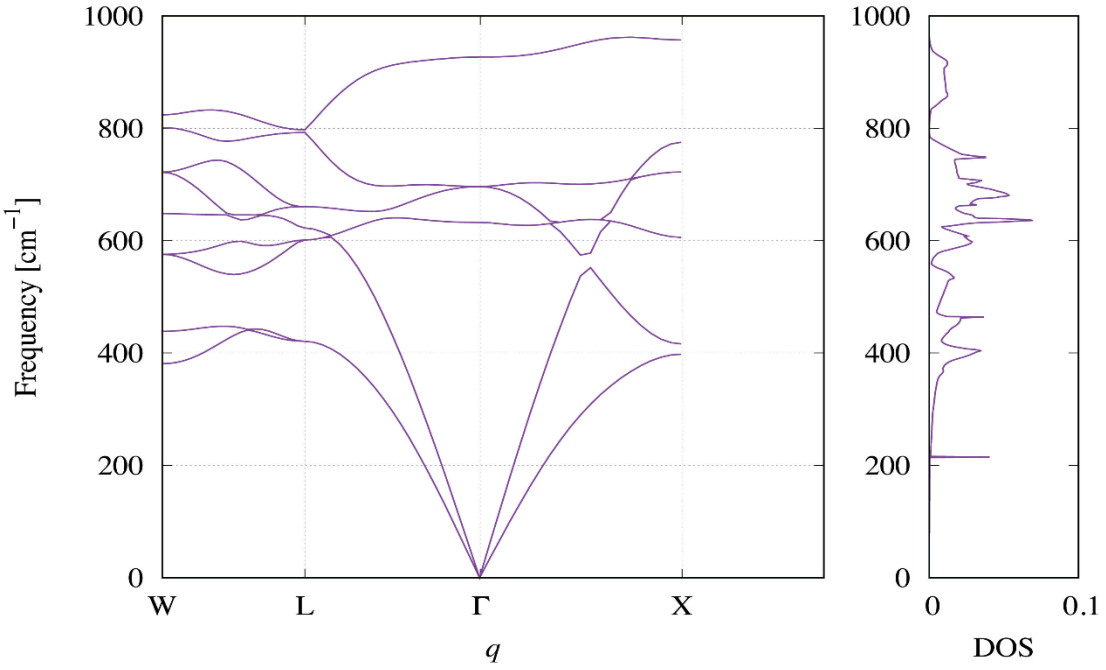

Fig 2: Phonon dispersion curve and phonon DOS for Be_2C.

Conclusion

A first principle DFT method has been implemented to investigate phonon properties of Be_2C. The lattice parameter at equilibrium is in good agreement with experimental data and previously calculated for Be_2C. The dispersion curve is characterized by absence of imaginary frequencies and hence the compound is dynamically stable. There are many research work on Be_2C related to structural, electronic and optical properties. This work on phonon properties is uniquely computed and hence this study can be helpful for further research on this crystal.

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