11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

Elastic, electronic and lattice dynamical properties of SiC

V. Ludwig(1)*, Z. M. da Costa Ludwig(1), M. J. Bell(1) and V. C dos Anjos(1)

(1) Universidade Federal de Juiz de Fora, Departamento de Física, ICE, cep 36036-330 , Juiz de Fora, MG, ludwig.valdemir@gmail.com.

* Corresponding author.

Abstract – We present theoretical results for elastic, electronic and lattice dynamical properties calculated using ab inito simulation program Siesta, based on the density functional theory approach. A comparison with experimental data from Rama measurements is given.

Recently, there has been intense interest in wide band-gap semiconductors due to potential applications in blue/UV optoelectronic and high power, high temperature, and high frequency electronic devices. SiC has proved to have in principle many advantages over other semiconductors [1]. At present, a few of the great variety of SiC polytypes, especially 3C, 4H and 6H are being considered for practical use in fabrication of micro-sensors. Despite a considerable interest in the studies of elastic properties of SiC pilytypes, we performed calculations to investigate elastic, electronic and lattice dynamical properties of SiC-3C polytype (fig. 1 and fig. 2).

We performed our ab initio calculations, based on norm-conserving pseudopotentials and density functional theory. The local density approximation (LDA) approximation has been used. The forces on the atoms are obtained form the Hellman-Feynman theorem and used form lattice dynamical calculations connection with Phonon code [2]. Firstly the equilibrium lattice parameters have been computed by minimizing the crystal total energy calculated for different values of lattice parameter.

Same basic physical properties, such as lattice constant, bulk modulus, cohesive energy and phonon frequencies and same band structural parameters are calculated and compared with those obtained with other recent theoretical works and in agreement with available experimental results [3].

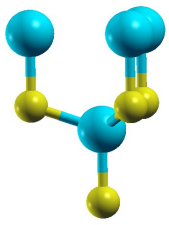

Figure 1: Unit cell of SiC-3C in cubic packing.

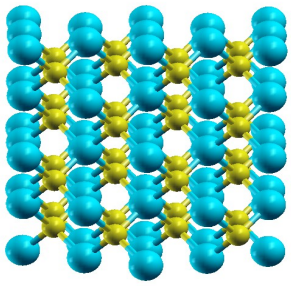

Figure 2: Supercell of 64 atoms used in our calculations.

References

[1]D. Nakamura, I. Gunjishima, S. Yamaguchi, T. Ito, A. Okamoto, H. Kondo, S. Onda & K. Takatori, *Nature* **430**, 1009-1012 2004.
[2]K. Parlinski, Software Phonon (2003) (and references therein)
[3]J. Serrano, et al. Physical Review Letters 98, 095503 2007.