J Material Sci Eng 2015, 4:3
http://dx.doi.org/10.4172/2169-0022.C1.032

OMICS International
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International Conference and Exhibition on
Mesoscopic & Condensed Matter Physics
June 22-24, 2015 Boston, USA

First principle calculations of the mechanical and electronic properties of hexagonal phase of BaF_2

P W O Nyawere[1,2], N W Makau[1] and G O Amolo[1]
[1]University of Eldoret, Kenya
[2]Kabarak University, Kenya

This is a presentation of electronic and mechanical properties of hexagonal phase of BaF_2 by First Principle methods. We have applied density-functional theory within generalized gradient approximation (GGA) using plane-wave pseudopotentials method and a plane-wave basis set. Our computed lattice parameter *a* is 4.269 Å comparable to experimental value of 5.516 Å (300 K) while the ratio of *b/a* in this work is at 1.4894 against experimental value of 1.297. The bulk modulus derived from the elastic constant calculations of hexagonal phase of BaF_2 is 161 GPa and value from Murnaghan methods is 154 GPa. The stabilities constants in various crystallographic directions are A_1 is 0.015 and A_2 is 0.023.

Biography

P W O Nyawere has completed his PhD from University of Eldoret through a Sandwich Training in Abdus Salaam International Center for Theoretical Physics, Trieste (Italy). Currently he is teaching Physics at Kabarak University – Kenya. He has published three papers in referred journals and one book *"Specific Heat Jump in High TC Superconductors"*. Currently, he is interested in First Principle Calculations of bulk materials.

pnyawere@gmail.com

New glasses; tellurite glasses

R El-Mallawany
Menofia University, Egypt

In materials engineering design prediction and understanding over the physical properties are essential to develop new class of functionalized materials. The modification of properties induced by the addition of transition metal oxides (TMO) or rare earth oxides (REO) into host glass matrix like tellurite glasses have attracted a lot of attention due to their physical properties and applications. The present work will throw some light on the structural aspects of these glasses. These quantitative conclusions will help in materials engineers and scientists to design, predict and understand the physical properties to develop new class of materials by calculations of:

- number of bonds per unit volume, nb,
- average stretching force constant in the glass network, $\overline{F}$,
- Calculated bulk modulus by bond compression model Kbc,
- ring diameter of glass network, ℓ,
- average crosslink density,
- Poisson's ratio, 6_{th}.
- for 26 composition of tellurite glasses

$$\overline{n}_c = \frac{\sum_i x_i (n_c)_i (N_c)_i}{\sum_i x_i (N_c)_i}$$

Biography

R El-Mallawany served as a research group leader for semiconducting tellurite glasses at Menofia University., Egypt. He published more than 90 international articles, taught physics for undergraduates & postgraduates for nearly 4 decades and supervised and examined 25 PhD & MSc thesis at 9 Egyptian & Arab Universities. Also, he cooperated with 15 American, European and Asian Universities in the experimental & theoretical contribution in optical, electrical, thermal, elastic and vibrational aspects in condensed matter physics "Semiconducting Glasses".

raoufelmallawany@Yahoo.com