Journal of
Materials Engineering and Applications

Abstract

Behavior of System Temperature of ZnO under the Effect of Pressure a Molecular Dynamics Prediction

Yahia Chergui

Badji Mokhtar University, Sidi Ammar, Annaba 23000, Algeria

Abstract:

Zinc oxide is a promising semiconductor, due to the chemical bonds; they are between covalent and ionic liaisons. This bonding plays a dramatic role in thermodynamic properties, under extended pressure and temperature. In this work, we analyze the behavior of the effect of pressure on the system temperature of ZnO wurtzite structure; we have been investigated equilibrium parallel molecular dynamics technique and dlpoly_4 software, using RAVEN supercomputer of Cardiff University(UK), to simulate the evolution in time of system temperature and its equilibrium time in isothermal and isobaric ensemble. Our system contains 2916 atoms of ZnO wurtzite type, under the ranges of pressure 0-200(GPa) and temperature 300-3000(K), where the interatomic interactions are modeled by Buckingham and Coulomb potential for short and long-range interactions respectively. Due to the lack of information about the effect of pressure on system temperature, under previous conditions, our results are still a prediction, which needs experimental confirmation in future. The thermodynamic behavior of ZnO has huge importance in nanoscale and macroscale, especially in medicine, pharmacy and geophysics fields.

It not only preserves its internal energy but multiplies it, at the expense of sucking in the energy of the environment. Thus the acceleration process turns to generation process . Because of the technical generation of this accelerating field is very complicated for now, it is necessary to imitate it using our well-known Electromagnetic field. The secret is in very unique shape of the input (to the antenna) electrical signal. It is imitated the accelerating signal using the well-known Electromagnetic field, that sucks the free cross vortices from the environment.

Biography:

Yahia CHERGUI is a lecturer in Electrical & Electronics Engineering Institute, Boumerdes Algeria. He has completed his PhD from Badji Mokhtar University in Annaba, Algeria. He did all his PhD work in Cardiff University in UK. His research field is Physics(condensed matter, simulation by molecular dynamics). He has many published articles and international conferences.

Recent Publications:

1. Y. CHERGUI, N. Nehaoua and D. E. Mekki Chapitre Solar Cells / Book 2 (first editin July 2011, InTec), ISBN979-953-307-191-5. Comparative study of dye-sensitized solar cell based on ZnO and TiO2: parameters evaluation, Edited by Prof. Leonid Kosyachenko Yuriy Fedkovych Chernivtsi National University, Optoelectronics Department, Ukraine.
2. N. Nehaoua, Y. CHERGUI and D. E. MEKKI Chapitre Solar Cells / Book 3 (first edition July2011, InTec), ISBN 9-953-307-192-2 A New Model for Extracting the Physical Parameters from I-V Curves of Organic and Inorganic Solar Cells Edited by Prof. Leonid Kosyachenko Yuriy Fedkovych Chernivtsi National University
3. Y. CHERGUI, N. Nehaoua and D. E. Mekki, Low and wide gap organic solar cells parameters extraction from illumination current-voltage. Materials Science, Trade Science, MSAIJ, 8(4), 2012 [174-178]
4. Y. CHERGUI, N. Nehaoua et D. E. Mekki, Photovoltaic characteristics of ZnO Nanotube Dye-Sensitized Solar Cells and TiO2 Nanostructure, Journal of Material Sciences,Issue 2321-6212, Page 2347-2278. 2/10/2013

Citation: Yahia Chergui Behavior of System Temperature of ZnO under the Effect of Pressure a Molecular Dynamics Prediction, Green Energy and Material Science, September 24, Dubai, UAE