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Radial Distribution Functions of ZnO Rocksalt and Zinc Blend Types a Molecular Dynamics Computation

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Parallal Molecular Dynamics and DL_POLY_4 software are used to analyze the pair correlation functions of ZnO rocksalt and zinc blend structures under different pressures and temperatures. Our system is formed from 5832 atoms of ZnO for rocksalt and zinc blend , the interatomic interactions are modeled by Coulomb-Buckingham Potential for short and long-range, the range of temperature is 300-3000K and for pressure is 0-100GPa. In this work we use radial distribution function to canculate the value of chemical bonds of Zn-Zn, Zn-O, and O-O under previous conditions of pressure and temperature. Although no more data under previous conditions our results are in the vicinity of available experimental and theoretical information. This work is very important in nanoscale of time and space and in different sectors of industry.

Key words: ZnO, pressure, temperature, energy, simulation, MD

Biography

Yahia CHERGUI is an assistant Professor 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, and soft matter simulation by molecular dynamics). He has many published articles and international conferences. He has been serving as a referee with condensed matter journal (IOP), Energy journal (Elsevier), and American Journal of Modern Physics.

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