A First-Principles Computational Study of Structural and Elastic Properties of ZnO

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ZnO has numerous uses in electronics. For example, ZnO has been studied as a candidate material for use in LEDs, n-p junctions, and Al/Au ohmic contacts. There has been recent interest in Al-doped ZnO for its thermoelectric properties. This is because this material possesses a high Seebeck coefficient, which measures the electrical potential generated by applying a thermal (temperature) gradient. The structural stability at temperatures above 1300 °C allows ZnO to be used as a high-temperature thermoelectric generator.

Several past studies have been referenced for the present work. The first focus of this study, there is a multitude of publications on ZnO that address its potential uses in many other areas of science and technology. In the next box on the right, we list several other applications of ZnO.

Method

The primary tool used in this paper is the Vienna Ab Initio Simulation Package (VASP), which is based on the density functional theory (DFT) to calculate the ground-state property of a substance. There are three known phases of ZnO, namely wurtzite (W), rock salt (RS), and zinc blende (ZB). The initial step is to determine the transition pressure for the structural transformation between the ZnO phases. This helps set a clear distinction between the high-pressure and ambient-pressure calculations. The second step is to obtain the bulk modulus. To calculate the bulk modulus, each structure is placed under a series of uniform pressure values. The resulting data are then fitted against the Birch-Murnaghan Equation of States (EoS). The third step is to calculate the elastic constants. The W structure is a hexagonal closely packed lattice. The RS and ZB phases have cubic lattices. To calculate the elastic constants, distortions are applied to the lattice. By using the difference in energy between the distorted and undistorted structure, the elasticity of the structure can be calculated.

Results & Discussion

Transition Pressure & Bulk Modulus


The transition pressure from figure 1 gives a clear distinction between high and low pressure calculations. The high pressure calculations were done at 15 GPa. By using a direct derivative method, we calculated the bulk modulus for the high pressure ZnO structures. The resulting bulk moduli are 193, 229, and 192 GPa for the W, RS, and ZB phases, respectively.

Conclusions & Further Study

The present work predicts a structural transition from the wurtzite to RS phase of ZnO at 11 GPa. We therefore performed high-pressure calculations at 15 GPa. The bulk moduli for the ambient-pressure structures are within 5% of previously reported results. Our calculations indicate that the high-pressure bulk moduli of ZnO phases increase between 38% and 56%. The RS and ZB phases of ZnO show increasing values of elastic constants C_{11} and C_{12} at higher pressure, while the value of C_{44} decreases at higher pressure. On the other hand, the wurtzite phase shows all increased elastic constants with increasing pressure. A comparison was made between the elastic constants of the ZnO phases and those of silicon. With the exception of C_{11} and C_{44} in the wurtzite phase, the three phases of ZnO exhibit higher values of elastic constants, indicating their higher strength under structural deformation. An important topic for future study of ZnO is to explore the electronic band structure and phonon dispersion, which will determine the properties crucial in many device applications. The structural results obtained in this work have laid a key foundation for continued research.