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Ab Initio Calculations of Structure and Elastic Properties of BexZn1−xO Alloys

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Abstract : There is a growing interest in Zn1-xBexO (ZBO)/ZnO hetero structures and quantum wells since the band gap energy of Zn1-xBexO solid solutions can be turned over a very large range (3.37–10.6 eV) as a function of the Be composition. ZBO/ZnO has been utilized in ultraviolet light emission diodes and lasers, and may find applications as active elements of various other electronic and optoelectronic devices. Band gap engineering by Be substitution enables the facile preparation of barrier layers and quantum wells in device structures. In addition, ZnO and its ternary alloys, as piezoelectric semiconductors, have been used for high-frequency surface acoustic wave devices in wireless communication systems due to their high acoustic velocities and large electromechanical coupling. However, many important parameters such as elastic constants, bulk modulus, Young's modulus and band-gap bowing. First-principles calculations of the structural, electrical and elastic properties of Zn1-xBexO as a function of the Be concentration x have been performed within density functional theory using norm-conserving pseudopotentials and local density approximation (LDA) for the exchange and correlation energy. The alloys' lattice constants may deviate from the Vegard law. As Be concentration increases, the elastic constants, the bulk modulus and Young's modulus of the alloys increase, the band gap increases with increasing Be concentration and Zn1-xBexO alloys have direct band. Our calculated results are in good agreement with experimental data and other theoretical calculations.

Keywords : DFT calculation, norm-conserving pseudopotentials, ZnBeO alloys, ZnO
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