Phase separation and interatomic distances in semiconductors with oxygen in the anion sublattice

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Semiconductor compounds with oxygen in the anion sublattice, such as CdO, ZnO, MgO, BeO and their ternary alloys (CdZnO, BeZnO, MgZnO), attract a very high attention in the last years due to wide perspectives for modern opto- (especial for green spectral region) and microelectronics [1-4]. However, their specific properties and tendency to phase separation (both composition fluctuations and several crystal phase coexisting) produce many problems with reproducible growth of materials, based on these ternaries compounds and, consequently, with application to practice [5]. Additionally, there is a lack of experimental and theoretical works on structural (including interatomic distances) and thermodynamic properties of these semiconductor alloys.

In the paper, we present the analysis of the structural (anion-cation, cation-cation and anion-anion distances) and thermodynamic properties (mixing energy, interaction energy and phase diagrams) of wurtzite and zinc-blende $Zn_xCd_{1-x}O$, $Zn_xBe_{1-x}O$ and $Zn_xMg_{1-x}O$ as a function of composition "x".

To find the structural and thermodynamic properties dependence on a function of composition "x", the simulations have been carried out with the modified valence force field method. The use of multiple computation runs was used to improve the representative statistics of the valence force field computations, which is necessary for an accurate prediction of properties and their composition dependences [6].

The interaction parameters of these compounds varies with the composition and can be well approximated by the second-order polynomial. This indicates that even the model of sub-regular solution is inadequate to account for the thermodynamic properties of these ternaries.
The phase diagrams of CdZnO computed on the basis of the thermodynamic properties derived from the valence force field simulations and the statistical model [6] exhibit asymmetry of the binodal spinodal curves with respect to the composition 50%.

Good agreement with the experimental data was demonstrated.

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