

Physical properties and Chemical bonds in the wurtzite- and zincblende-type structures.

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The relationship between the physical properties and chemical bonds in the wurtzite- and zincblende-type structures is discussed experimentally. The wurtzite- and zincblend type structure are classified tetrahedrally coordinated covalent compounds. These two structures have the same environment of the first and second nearest neighbors but different environments of the third nearest neighbors. The electrostatic interaction between an atom and its third neighbors in the wurtzite type structure is greater than in zinkblend. In addition to the difference in the configuration of distant neighbors, the lower symmetry of the wurtzite type structure allows for a distortion along the c axis away from the regular tetrahedral bond distribution. For most of the compounds with wurtzite structure, the apical bond distances are longer than the basal ones. This is due to the electrostatic attraction and/or the difference in the contribution to hybridization between three direction and another symmetrically non-equivalent direction. From the crystallographical viewpoints, the covarently bonded both type compounds show a systematic tendency towards lattice instability as ionicity increases. This lattice instability and thermal conductivity correlate to the anharmonic thermal vibration of atoms. The strengthes of the covalent bonds in stable wurtzite type compounds are decreased with increasing ionicity. The covalent compounds with moderate ionic character such as ZnO retain great stability and desirable chemical bonding character for wurtzite type structure. Divergent-like curves of the magnitudes of the mean-square displacement and mean-square relative displacement of both compounds are observed and indicates the behavior of lattice instability. Super ionic conduction generates a broad interatomic potential and strongly correlated displacement in thermal vibration between cation and anion.

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