Universality of the Empty-Lattice Approximation to Predict the Topology of Energy Spectra of High-Symmetry Crystals and Superlattices Based upon Them

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The idea of a relation between the elementary energy bands resulting from the empty-lattice approximation and the spatial valence electron distribution was proved up to now for semiconducting orthorhombic crystals and some consequences of this relation were stated [1,2]. Here it is demonstrated that there are no restrictions to use the results of the empty-lattice approximation concerning the selection of the actual Wyckoff position that is responsible for a spatial valence electron distribution in a unit cell. For this purpose we consider the basic crystals from A\textsuperscript{IV} (Si, Ge), A\textsuperscript{III}B\textsuperscript{V} (GaAs, AlAs), A\textsuperscript{II}B\textsuperscript{VI} (CdTe), A\textsuperscript{IV}B\textsuperscript{VI} (PbS) groups and superlattices based upon A\textsuperscript{IV} and A\textsuperscript{III}B\textsuperscript{V} crystals.

The investigation results show a surprising efficiency of this simplest approximation in the solid state theory. In particular, this approximation recognizes the energy states in the real valence band of the crystals and of superlattices mentioned above. Those energy states, described in the framework of the elementary energy bands concept, [3] have a close relation to the distinguished Wyckoff positions which are the centers of the valence electron density for crystals and superlattices. By considering the decrease of the symmetry from O\textsubscript{h}\textsuperscript{7} to T\textsubscript{d}\textsuperscript{2} groups, describing e.g. Si and GaAs crystals, the so-called itinerant Wyckoff position was found along the line connecting the nearest neighbors in the unit cell. This itinerant Wyckoff position has its equivalence in the unit cell of a superlattice.

A possibility for the creation of the valence band of a crystal and of a superlattice with the account of the energy states induced from the local groups of two or more Wyckoff positions was also observed. A fast method to predict a chemical bonding even in the case of a complicated crystal was proposed. The obtained information can be used to predict a localization position of a dopant in the unit cell as well as the structure of a solid solution.