A review of the structural, electronic and elastic properties of spinels

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The crystals with the spinel structure form a large group of technologically important materials. The spinels with the halogen atoms as the anions are typical semiconductors with a narrow band gap, whereas the oxygen-based spinels possess considerably wider band gaps, which make them suitable for doping with rare earth and transition metal ions. In the present work a review of the structural, electronic, optical and elastic properties of a large group consisting of 185 ternary and binary spinel compounds is given. At first, a simple empirical model based on the ionic radii and electronegativities of the constituting ions was developed [1]. The average relative error between the experimental and modeled lattice constants is less than 1 %. The model allowed for a prediction of the lattice constants of new spinels [1]; moreover, the criteria of stability of spinel structure were suggested that can be used for narrowing the search space when looking for new spinels. As a further step, the ab initio and semi-empirical methods were used to analyze the electronic, optical and elastic properties of pure and doped spinels, like $ZnAl_2S_4$, $ZnGa_2O_4$ [2-4], $CdIn_2S_4$ [5]. Special attention was paid to the location of the impurities energy levels within the host band gap; suggested combination of the semi-empirical and ab initio techniques gives a complementary description of doped materials.

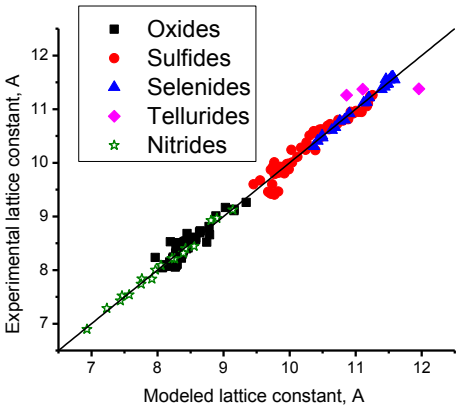

Fig.1. Correlation between the modeled and experimental lattice constants in the group of 185 cubic spinels, which were classified according to the anions (oxides with O, sulfides with S, selenides with Se, tellurides with Te, nitrides with N).

References

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