Lattice constant prediction of A_2XY_6 cubic crystals (A = K, Cs, Rb, Tl; X = tetravalent cation; Y = F, Cl, Br, I) using computational intelligence approach

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Abstract:

Lattice constant mismatch between materials affects the quality of thin film fabrication. For this reason, lattice constants information is vital in the design of materials for technological applications. The determination of lattice constants via experimental analysis is relatively expensive and laborious. As a result, several linear empirical models have been proposed to predict the lattice constant of crystal structures. However, the accuracies of these models are limited partly due to their failure to account for nonlinearity in the atomic parameters-lattice constant relationship. Machine learning techniques have shown excellent ability to deal with nonlinear problems in many areas of materials science; hence, they are considered suitable computation tools to study the crystal structure of materials. In this contribution, we developed a support vector regression (SVR) model to predict the lattice constant of cubic crystals of the form A_2XY_6 (A = K, Cs, Rb, TI; X = tetravalent cation; and Y = F, Cl, Br, I). The SVR algorithm uses the ionic radii and electronegativities data of the constituent elements of A_2XY_6 cubic crystals as model inputs. The robustness of the proposed model was demonstrated by comparing our result with an existing linear model based on 26 cubic crystal samples. The result revealed a total relative deviation of 1.757 and 2.704 for the SVR model and the existing linear equation, respectively. This result proves that the SVR model has a huge potential in the search for new materials for different applications.

Keywords: Lattice, Constant prediction, A2XY6 Cubic Crystals, (A = K, Cs, Rb, TI; X = tetravalent cation; Y = F, Cl, Br, I), Computational intelligence

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