Diffusion Path Formation for Cu^+ Ions in Superionic Cu_6PS_5I Single Crystal

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The knowledge of structural transformations to phases characterized by high ionic conductivity remains still very important in understanding the mechanisms and structural conditions supporting high mobility of ions in solids.

Trying to understand the mechanism for superionic conductivity of Cu^+ ions in Cu_6PS_5I argyrodite compound the detailed structure analysis based on single-crystal X-ray diffraction was performed. The main interest was focused on a new cubic superstructure F-43c, stable from 140K to 275K. In the range of this phase ordering of copper ions occurs. The final structure model is given including the detailed temperature evolution of site occupation factors of copper ions. Possible diffusion paths for the copper Cu^+ ions are represented by means of the atomic displacement factors and split model. Ordering process of Cu^+ ions with temperature lowering is found to be similar with ordering of copper in β-Cu_7PSe_6 [1].

Comparison of the structural data with non-Arrhenius behavior of conductivity [2] indicates significant change in conduction mechanism with temperature increasing: from hopping to liquid like behavior.

[1] Gaudin E., et al., *Acta Cryst*., 2000, B**56**, 402-408. [2] Beeken R.B., et al., *Journal of Physic and Chemistry of Solids,* 2003, **64**, 1261-1264.

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