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X-ray Study and Computer Simulation of the Structure of Amorphous-Crystalline Titanite

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The structure of amorphous-crystalline titanite obtained by mechanical activation was studied by X-ray diffraction and simulation methods. The short-range order characteristics were calculated using Finbak–Warren's method. It was found that the coordination numbers of metal atoms decreased as the result of titanite grinding. The atomic configurations of short-range order of ground titanite were constructed by translation of titanite unit cell. The theoretical X-ray patterns were calculated using Debye's method and were compared with the experimental curves. The structure of ground titanite in the mill with centrifugal factor 40 g was described satisfactorily by the model of mechanical mixture of clusters containing 2016 atoms, disordered during the molecular dynamics with clusters containing 12096 atoms. The increase of grinding intensity led to the sharp decrease of sizes of small cluster.

Keywords: amorphous-crystalline titanite, X-ray diffraction, computer simulation, mechanical activation, Debye's method.