MODELING OF THE OXIDE MELT STRUCTURE: GLASS TRANSITION VS CRYSTALLIZATION

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Due to the increasing demand for the quantitative description and investigation of various processes in oxide systems, the creation of models of multicomponent melts, glasses, and their crystallization products is an extremely relevant task. Although glasses possess an unusual combination of properties that are in many ways closer to liquids than to true solids, on a human timescale they also demonstrate hardness, elasticity, and even fracture like solids. Given that crystalline materials preserve their internal structure and external configuration even for an infinitely long time and do not undergo plastic deformation at low temperatures under the influence of gravity, they are considered as real solids.

The present work is based on a thermodynamic description of the melt phase, which allows us to determine the conditions of the melting and differentiation processes, as well as to develop various methodologies for use in materials science and geological research. Using the quasicrystalline approximation based on the assumption that melts are composed of ideal associated solutions, the thermodynamic characteristics of crystalline silicates can be applied to describe the melt structure in terms of the distribution of Q^n units. It is known that silicate melts contain disordered polymerized anions which form the structural units of glasses and crystalline silicates. These consist of silicon–oxygen tetrahedra Q^n, which differ in the number of non-bridging and bridging oxygen atoms (n), with a central silicon atom and four oxygen atoms

The thermodynamic modeling method, which has proven highly effective for modeling melts at different temperatures, is used for the calculation of glass structure in this work. Since the melt and glass crystallization model is still under development, we used DFT analysis calculations. The structure of oxide melts, glasses, and crystals lends itself well to analysis using Raman spectroscopy. Since calculations of structure or chemical composition must be validated experimentally, this study demonstrates the potential of computational methods in comparison with experimental results. A qualitative comparison between theory and practice glass formation and crystallization of silicate melts containing equal amounts of lithium and potassium, with a total content of 33, 40, and 50 mol % was carried out using the methods of spectroscopy and X-ray diffraction.

This work was supported by the grant of the Russian Science Foundation No. 25-17-20015 (https://rscf.ru/project/25-17-20015/).