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The structure of bulk Al₂O₃ glass

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Alumina (Al₂O₃) has many applications, e.g., in cements, substrates of electronic materials, and high-temperature crucibles. Alumina can be classified as an intermediate between glass formers and modifiers, according to Sun [1]. It is impossible to prepare bulk alumina glass by using the melt quenching method and hence electrochemical and sol-gel methods were used to prepare the samples for studying optical properties and the behavior at high temperatures. However, the structure of alumina glass is still largely unknown due to the very limited number of structural studies.

In this study, we performed high-energy X-ray and neutron diffraction measurements on bulk alumina glass prepared by the electrochemical method. To understand diffraction data in detail, we employed a combined classical molecular dynamics-reverse Monte Carlo modelling approach, with coordination number constraints based on NMR data. The formation of OAl₃ triclusters could be confirmed. Detailed topological analyses are in progress.

[1] Sun, K. H. (1947). J. Am. Ceram. Soc. 30, 277.

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