Using molecular dynamics to descend into the structural complexity of EuF3 doped ZrF4-BaF2-LaF3-AlF3-NaF (ZBLAN) glass

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Abstract

The ZrF4-BaF2-LaF3-AlF3-NaF (ZBLAN) family of fluorozirconate glasses was developed due to the ease with which lanthanides can be incorporated for optical applications. The ZBLAN glasses are also interesting because they do not have a close analogue among other glass forming systems. As in oxide glasses the short range order is based on smaller cations surrounded by larger anions, but ZBLAN glasses do not follow the Zachariasen rules. Here we present a detailed classical molecular dynamics modelling of a series of ZB, ZBL, ZBA, ZBN, ZBLA and ZBLAN glasses. This methodology helps to identify the short range order and structural role relevant to each cation. The culmination is a 100A size model of Eu doped ZBLAN glass of relevance for optical applications.
The structural units of binary fluorozirconate glasses were carefully studied as they do not follow the Zachriasen glass model. The coordination number for

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