Local order around rare earth ions during the devitrification of oxyfluoride glasses

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Auteur	Silva, Maurício A.P. [1], Dantelle, Géraldine [2], Mortier, Michel [3], Monteil, André [4], Ribeiro, Sidney J.L. [5], Messaddeq, Younes [6], Briois, Valérie [7], Poulain, Marcel [8]
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Résumé en anglais	Erbium L(3)-edge extended x-ray absorption fine structure (EXAFS) measurements were performed on rare earth doped fluorosilicate and fluoroborate glasses and glass ceramics. The well known nucleating effects of erbium ions for the crystallization of cubic lead fluoride (based on x-ray diffraction measurements) and the fact that the rare earth ions are present in the crystalline phase (as indicated by Er(3+) emission spectra) seem in contradiction with the present EXAFS analysis, which indicates a lack of medium range structural ordering around the Er(3+) ions and suggests that the lead fluoride crystallization does not occur in the nearest neighbor distance of the rare earth ion. Molecular dynamics simulations of the devitrification process of a lead fluoride glass doped with Er(3+) ions were performed, and results indicate that Er(3+) ions lower the devitrification temperature of PbF(2), in good agreement with the experimental results. The genuine role of Er(3+) ions in the devitrification process of PbF(2) has been investigated. Although Er(3+) ions could indeed act as seeds for crystallization, as experiments suggest, molecular dynamics simulation results corroborate the experimental EXAFS observation that the devitrification does not occur at its nearest neighbor distance.
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