Molecular dynamics simulation of an erbium-activated titania-silica glass: composition influence on the structural properties

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Résumé en anglais	We have performed molecular dynamics simulations of a TiO2–SiO2: Er3+ system for various compositions. Different distribution functions have been analysed to determine whether titanium ions are homogeneously distributed. A similar analysis has been carried out to characterize the erbium clustering ability. In particular, because of the simulation technique, the microscopic structure around erbium ions has been investigated. We discuss the role of both erbium and titanium concentrations in the structural properties of the simulated samples. For this purpose, the titanium distribution has been studied for [Ti]/[Si + Ti] concentrations ranging from 7.8 to 50% in undoped samples, and the erbium clustering trend has been characterized from three doped samples in which both erbium and titanium concentrations vary. A calculation of the crystal-field strength for the different kinds of erbium site has been interpreted in the light of the associated local structures.
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Liens

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