Structural study of TeO2-MyOz glasses by X-ray total scattering and molecular dynamics

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Abstract

Tellurite materials, especially in their vitreous forms, are of major interest in the field of information and communication technologies due to their remarkable optical properties. Pure tellurium dioxide TeO2 glass shows important non linear susceptibility and Raman amplification superior to that of silicon-based glasses. However, its thermal stability and its poor mechanical properties make it difficult to use the pure TeO2 glass as it is. Adding a modifier to compensate for the drawbacks without degrading the optical properties becomes a necessity. In order to understand the evolution of the properties with the addition of a modifier, the structural study of the modified glasses, in comparison with the pure glass, is essential.
This study consists of two sections: an experimental part put in comparison with a simulation of the glasses structures. The modifiers were chosen to be a transition element oxide and an alkali element oxide in order to be able to study the influence of the type of modifier and its quantity on the glass structure.

After the synthesis of pure TeO2 glass and (100-x)TeO2-xMyOz (with M the alkali or the transition element) samples, structural studies based on experimental techniques, such as X-ray diffraction and Raman spectroscopy, were led in order to verify the amorphous nature and the homogeneity of the samples. Thermogravimetric analyses were realized to follow the evolution of the thermal stability of the glasses with the addition of modifier. An X-ray total scattering study was completed to determine the changes in the environment of the Te and O atoms in the glasses by comparing the pair distribution functions (PDF) of the different samples.

The simulation of the structure was carried out using the DL_POLY [1] software using interatomic potentials for Te-O [2] and M-O [3]. PDF were calculated based on the simulated structures and were compared to the experimental ones.

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