Structure of Telluride Glasses: a Theoretical and Spectroscopic Investigation

Claudia Gonçalves[1], Marc Dussauze*[2], Raphael Mereau[2], Eric Furet[3], Deschamps Michael[4], Virginie Nazabal[1], Catherine Boussard-Pledel[1], and Bruno Bureau[1]

[1]Institut des sciences chimiques de Rennes, UMR-CNRS 6226, – Laboratoire de Sciences Chimiques, UMR-CNRS 6226, Université de Rennes 1 – France

[2]Institut des Sciences Moléculaires (ISM) – Centre National de la Recherche Scientifique - CNRS : UMR5255, Université de Bordeaux (Bordeaux, France) – Bâtiment A 12 351 cours de la Libération 33405 TALENCE CEDEX, France

[3]Institut des sciences chimiques de Rennes, Ecole Nationale Supérieur de Chimie de Rennes – Laboratoire de Sciences Chimiques, UMR-CNRS 6226, Université de Rennes 1 – France

[4]CEMHTI, CNRS UPR 3079, université d'Orléans – Centre National de la Recherche Scientifique - CNRS – France

Abstract

The central goal of our project is to rationalize the substituent effect on the glass structure and physical properties of a new generation of far-infrared transmitting telluride materials. Indeed the research area is nowadays receiving an increased attention because of the various potential photonic-related application, like monitoring, night vision, and CO2 greenhouse effect monitoring1. Due to the lack of long-range order in glasses, structural characterization is always a challenge. Spectroscopic techniques probing the local environment of selected atoms, such as solid-state NMR, is a well-known approach to understand the structural and physical properties of new families of glasses. Another way to get structural and dynamical insights of our materials are the use of structural characterization by IR/Raman vibrational spectroscopies. In this study, an accurate structural characterization of ternary glasses in the systems Ga-Ge-Te and Ge-Te-Se is presented. The NMR study has been carried out using quite unusual nucleus like 73Ge, 77Se, 125Te and 69/71Ga. For instance, the 73Ge nucleus, which is a very low-gamma nucleus with a large quadrupolar moment, needs to be probed using a high magnetic field spectrometer. Besides, results of vibrational spectroscopies will be shown for the two families of telluride glasses, a careful assignment of vibrational modes is proposed thanks to DFT calculations implemented using the Gaussian software.

Keywords: telluride glasses, NMR, infrared, Raman, DFT calculation

*Speaker