Structure and crystallization in the B2O3-La2O3 binary and focus on the congruent lanthanum metaborate composition (LaB3O6)

Hélène Trégouët[1], Erwan Chesneau[2], Odile Majérus*[1], Thibault Charpentier[2], Laurent Cormier[3], Daniel Caurant[4], and Hervé Vezin[6,5]

[1]Institut de Recherche de Chimie Paris (IRCP) – Paris Sciences et Lettres, Ecole Nationale Supérieure de Chimie de Paris – Chimie Paristech, 11 rue P et M Curie, 75005 Paris, France

[2]Laboratoire de Structure et Dynamique par Résonance Magnétique (LSDRM) – CEA-CNRS UMR 3299, – France

[3]Institut de minéralogie, de physique des matériaux et de cosmochimie (IMPMC) – Institut de recherche pour le développement [IRD] : UR206, Université Pierre et Marie Curie (UPMC) - Paris VI, CNRS : UMR7590, Muséum National d'Histoire Naturelle (MNHN) – Tour 23 - Barre 22-23 - 4e étage - BC 115 4 place Jussieu 75252 PARIS, France

[4]Institut de Recherche de Chimie Paris (IRCP) – Ecole Nationale Supérieure de Chimie de Paris – France

[6]Reseau sur le Stockage Electrochimique de l'Energie (RS2E) – Reseau sur le Stockage Electrochimique de l'Energie (RS2E) – 33 rue Saint Leu, 80039 Amiens, France

[5]Université Lille Nord de France – Université Lille Nord de France – F-59655 Villeneuve d'Ascq, France

Abstract

The B2O3-La2O3 binary system contains a narrow glass domain around the La2O3.3B2O3 metaborate composition. This glass domain is of interest in the field of nuclear waste containment glasses, rich in rare-earths and B2O3, and as optical materials. An extensive study of the structure and crystallization properties of these glasses has been undertaken recently1-3. In this paper, we focus on the lanthanum metaborate composition, that melts congruently at 1140∘C. When undercooled, the crystallization of this melt is characterized by a heavily heterogeneous nucleation and a high activation energy for the crystal growth (_˜ 800 kJ.mol-1). To understand these peculiar properties, we compare the crystal and the melt structures, using a range of complementary techniques. 11B and 17O MAS NMR results do not indicate significant differences regarding the fraction of fourfold coordinated boron and the fraction of non-bridging oxygens in the crystal and in the glass, while Raman (performed on a series of binary glasses around the LaB3O6 composition) reveals a complex borate network with a great variety of superstructural units, dissimilar to that of the crystal. RE sensitive spectroscopic tools such as optical spectroscopies (Nd3+ and Eu3+ substituted for La3+) and EXAFS pointed out shorter RE3+-NBO interactions in the glass. X-ray wide angle (WAXS) and neutron scattering measurements have been carried out to produce the total structure factors and allow the building of structural models for the glass, allowing a deeper insight into the differences and relationships to the crystalline structure.

*Speaker

1 O. Majérus, H. Trégou´et, D. Caurant, and D. Pytalev, *J. Non. Cryst. Solids*, vol. 425, pp. 91–102, 2015.
2 D. S. Pytalev, D. Caurant, O. Majérus, H. Trégou´et, T. Charpentier, and B. N. Mavrin, *J. Alloys Compd.*, vol. 641, pp. 43–55, 2015. 3 H. Trégou´et, D. Caurant, O. Majérus, T. Charpentier, L. Cormier, and D. Pytalev, *Procedia Mater. Sci.*, vol. 7, pp. 131–137, 2014.

Keywords: Borate glasses, rare, earths, glass structure, crystallization