The structure of glasses and melts: order in the chaos

G. CALAS*, L. CORMIER AND L. GALOISY

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie - Sorbonne Universités - UPMC - CNRS -IRD - Muséum National d'Histoire Naturelle, F-75005 Paris, France

(*Correspondence: georges.calas@upmc.fr)

More disordered than nanomaterials, glasses and melts have benefited from molecular scale approaches, which provided a deeper knowledge of their structural organization and have given potential tools to predict glass/melt properties. We will summarize structural data obtained by structural (EXAFS, neutron and X-ray diffraction), spectroscopic (XANES, UV-visible, EPR...) and numerical modeling/simulation approaches, with an emphasis on the surrounding of cations, sensitive witnesses of the chemical diversity of these materials.

These approaches have given rise to dramatic progresses in the understanding of the structural properties of glasses and melts: existence of "exotic" coordination sites and of some medium range order, heterogeneous distribution of cations, etc... Recent in-situ data at high temperature provide a quantification of the thermal expansion of cation sites and illustrate structural modifications between glasses and melts. All these data show that bond valence rules and the principles governing mineral crystal chemistry are also acting in glasses and melts, emphasizing the interdependence between their local structural organization and the chemical state of glass/melt components.

Many structure-property relationships have been found in glasses, within a broad range of fields: crystalline nucleation, mineral activity in silicate melts, glass coloration, including that of historical glasses and the cultural heritage, or the prediction of the stability of nuclear waste glasses under forcing conditions (irradiation, alteration...). Glasses and melts, once referred to only as amorphous, show indeed a large diversity of their structural organization and of their properties.