

s12.m34.o3 **Characterising the Structural Disorder associated with Superionic Conduction in Crystalline Materials.** David A Keen^{a,b} and Stephen Hull^b, ^aDepartment of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford OX1 3PU U.K., ^bISIS Facility, Rutherford Appleton Laboratory, Didcot, Oxon OX11 0QX U.K. E-mail: d.keen1@physics.ox.ac.uk

Keywords: Molecular Dynamics; RMC; Superionic Conductors

Superionic conductors are materials with exceptionally high ionic conductivity whilst still in the solid state. Structural disorder is a natural consequence of this ionic mobility, associated with the movement of the conducting ions through the lattice. In superionic materials with the highest ionic conduction, this disorder can be very extensive, and average structural descriptions may not be very helpful for characterising this disorder. This is usually because the small number of observed Bragg reflections yield ambiguous split-site models of the disorder, which may additionally contain large anisotropic atom displacement parameters. Here we describe alternative approaches for describing the disorder, using combinations of molecular dynamics simulation, bond valence calculations and reverse Monte Carlo modelling of total scattering neutron diffraction data. By way of an example, we use an investigation of the superionic conductor Ag₃SI, a material with three distinct crystalline phases and an ionic conductivity which changes by over six orders of magnitude between 100K and 300K.

s12.m34.o4 **Characterization of Radiation-Damaged Materials by Means of Small-Angle X-Ray Scattering.** Susana Rios, Dept. of Earth Sciences, University of Cambridge, Great Britain. E-mail: rios@esc.cam.ac.uk

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Materials containing radioactive dopants often undergo a crystalline-to-amorphous transformation. The heavy recoil nucleus released during the radioactive decay will experience ballistic collisions with the surrounding crystalline matrix, leading to the production of amorphous cascades, and eventually to complete amorphization. Minerals, such as zircon (ZrSiO₄) and pyrochlores (A₂B₂O₇), contain uranium and thorium impurities, and are known to go amorphous over long periods of time. In the case of zircon, as the long-range order is gradually lost, nano-scale density fluctuations start to develop. The small-angle x-ray scattering (SAXS) signal is characterized by two distinct contributions. The first component relates to the surface scattering coming from relatively large crystalline regions that still survive the amorphization process. These regions, having a density 18% larger than the surrounding amorphous matrix are clearly observed by SAXS techniques [1]. The second contribution is associated to one nanometer size density fluctuations related to the topology of the amorphous phase [2]. In this presentation, the evolution of the SAXS intensity is shown as a function of temperature. For this purpose, two zircons with 85% and 100% amorphous content were selected, and annealed up to 1300 °C to achieve complete recrystallization. The origins of the SAXS intensity are discussed in terms of two possible scenarios: i) the existence of vacancy aggregates produced during the formation and subsequent percolation of amorphous cascades, and ii) due to damage-induced phase segregation (amorphous silica / crystalline zirconia). If the SAXS intensity originates from vacancy aggregates produced during cascade formation, this might be a common feature for ceramics undergoing similar amorphization processes. Recent diffusion experiments favour this hypothesis [3]. On the contrary, if density fluctuations are due to phase segregation, this phenomenon might be specific to systems where parts of the crystalline structure are able to accommodate the damage by producing highly polymerised structures. Results found in zircon are compared to recent studies performed in a series of α -decay damaged pyrochlores (Na, Ca)₂(Nb,Ta)₂O₇.

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