ESRF	**Experiment title:** Structural Modifications in Rare-Earth Metaphosphate Glasses at Low Temperatures	**Experiment number:** CH-725
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Report:

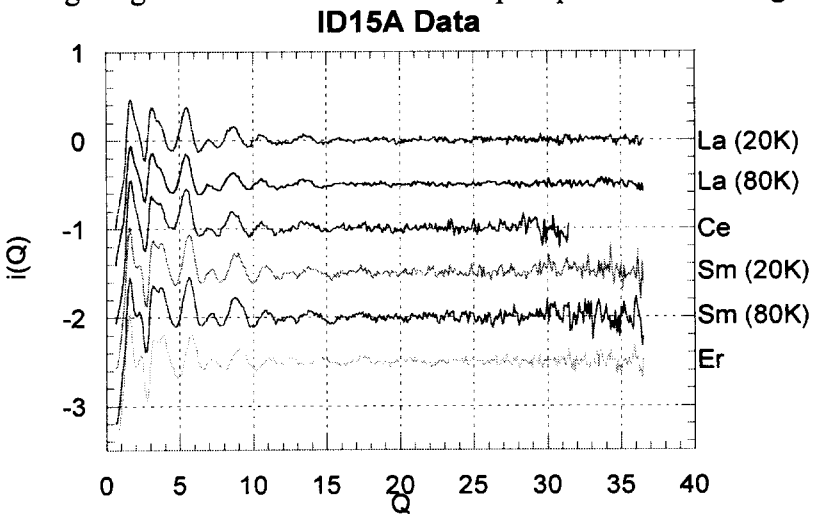
Rare-earth phosphate glasses (REPGs) of compositions $[(Ln_2O_3)_x(P_2O_5)_{1-x}$, x = 0.167-0.25] have shown great promise in the laser and optoelectronics industry. Furthermore, since the dopant rare-earth ions exist in such a high concentration (17-25% molar volume: Ln_2O_3) REPGs have also been found to exhibit a myriad of exotic thermal, acoustic and magnetic phenomena at low temperatures [1-3].

In an attempt to understand and thus optimise these physical properties, we have been investigating the atomic structure of the series of REPGs (where Ln = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er). Due to the high structural complexity of glasses, extensive use of a wide range of structural techniques (EXAFS, conventional X-ray and neutron diffraction, anomalous X-ray diffraction, NMR and IR) has been employed in order to build up a coherent structural picture of these compounds [4-7]. The high-energy diffraction experiment reported herein forms an integral part of this project. It also complements well analogous EXAFS work undertaken on station BM29.

Five REPG samples were studied in total: $(R_2O_3)_x(P_2O_5)_{1-x}$ where R = La, Ce, Sm, Er, Tm and x = 0.225, 0.197, 0.226, 0.239, 0.230 respectively. The Ce, Er and Tm samples were studied in their powder form at ambient temperature whilst measurements on the other two were carried out at low temperature (12K and 80K) using the bulk glass. All measurements utilised a wavelength of 0.10346Å (120keV) and a $2\theta/\theta$ set-up. There were no major problems with the experiment.

The data are presently being analysed and preliminary results have already been obtained. Structural information can be interpreted in real-space reliably up to a Q_{max} of $30Å^{-1}$, the whole data-sets extending to Q_{max}=$36.5Å^{-1}$. The use of nearly all of this range indicates that the data are very accurate. Figure 1 shows these results, from which one can see that structural features extend in Q-space much further than analogous results obtained via previous measurements at the Daresbury facility, UK, where an intrinsic Q_{max} limit of 18-

19Å^{-1}. Furthermore, this extensive Q-range compares well to analogous neutron diffraction data obtained on LAD at the ISIS facility where a Q_{max} = 50Å^{-1} was obtained [7]. Given this comparable Q-range, we are currently working on methodologies to exploit this complementarity in the fitting process, such that the correlations which have more favourable X-ray / neutron scattering factor weightings are treated accordingly. This approach will yield a significantly more accurate and comprehensive picture of the complex structure of REPGs. Figure 2 shows the real-space information derived from the X-ray and neutron data, thus illustrating the stark contrasts in X-ray and neutron weighting factors. In particular, the neutron data appear to be more suited to probe the correlations associated with oxygen, whilst the X-ray data evidently provide more weighting towards the rare-earth and phosphorus containing correlations.



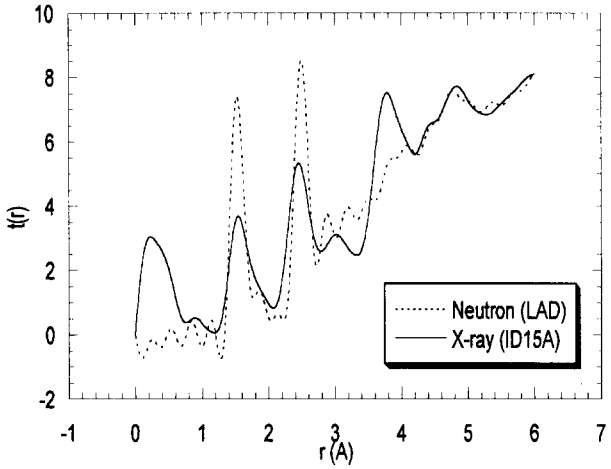


Figure 1: The intereference function, I(Q), for $(R_2O_3)_x(P_2O_5)_{1-x}$; Figure 2: A comparison between neutron and X-ray data for $(Ce_2O_3)_{0.197}(P_2O_5)_{0.813}$ with comparable Q-ranges.

The variable temperature measurements were undertaken in order to ascertain whether or not structural perturbations were responsible for anomalous physical properties that ensure below T = 20K [1-3]. Figure 3 shows the comparison between the 12K and 80K measurements for the Sm sample. Analogous results for the La data are similar. There is no discernible difference in structure with temperature and we thus conclude that the anomalous physical properties do not result from structural origins within the glass.

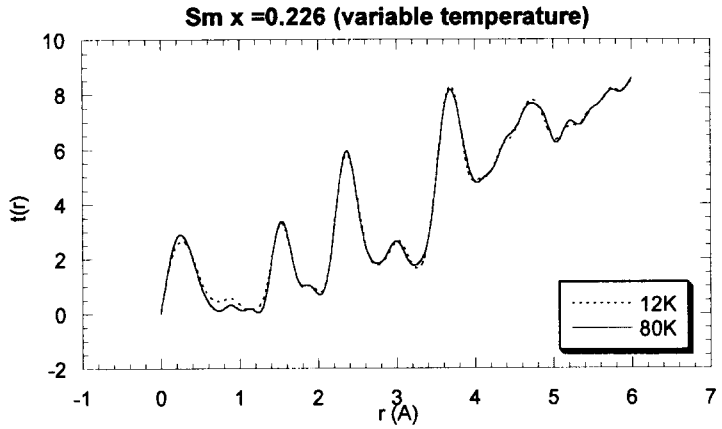


Figure 3: A comparison of the structure of $(Sm_2O_3)_{0.226}(P_2O_5)_{0.774}$ at 12K and 80K.

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