

MS017.P01

*High-accuracy Ni-doped borate-glass comparison using x-ray extended-range technique*Geoffrey Phillip Cousland¹, Redi Pingak¹, Christopher Chantler¹, Victor Streltsov¹, Stephen Best²¹School Of Physics, University Of Melbourne, Parkville, Australia, ²School of Chemistry, University of Melbourne, Parkville, Australia
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The x-ray extended range technique (XERT) has proven accuracy when used with crystal structures. With the advent of XERT, and with synchrotron x-ray radiation available at many facilities worldwide, many researchers already have the possibility of using this powerful tool for structure determination of crystals. An obvious question is the how this methodology can be extended to solve other structure-related problems. Here we show how to extend structure and function determinations to solving the structure of disordered Ni-doped borate-glasses which still, of course, have local order.

Borate glasses are useful for fibre-optic communication and non-linear optic applications, and have already been investigated for coloration, ferroelectric properties and second harmonic generation [1]. High-accuracy measurement of Ni-doped borate-glass can be used to investigate structure and test current structural theories, such as the 'crystallite' model and non-crystal structure theory [2]. To achieve this, a methodology requires not only accurate estimates of structure but, and perhaps more crucially, experimental datasets of high-accuracy.

New techniques developed by our group are used to obtain x-ray absorption fine structure datasets with an accuracy unobtainable until recently [3]. The x-ray extended range technique (XERT) developed by our group is applied to dilute, nickel-doped borate glass $x\text{Li}_2\text{O}:(1-x-y)\text{B}_2\text{O}_3 + y\text{NiO}$, where $x = 0.33$ and $y = 0.05$. This is one of the first studies developing the XERT for dilute systems and the first study using XERT for borate-glass.

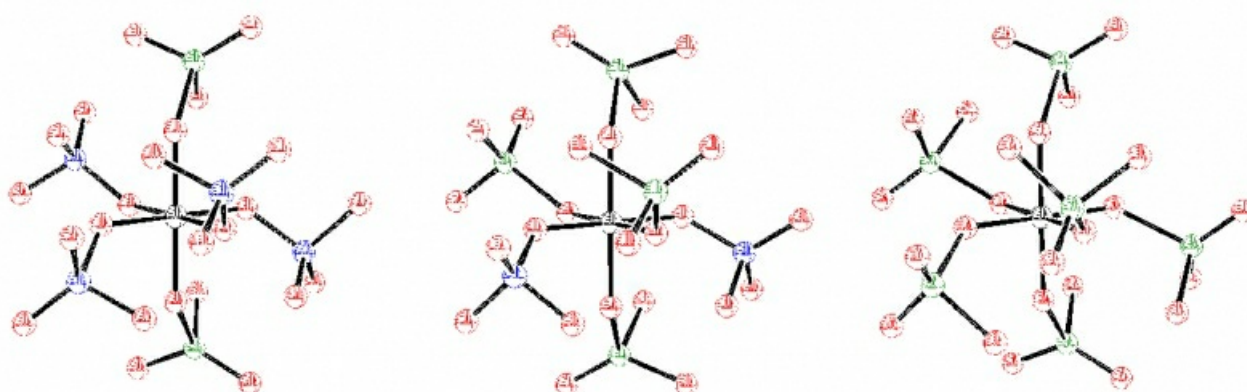
Datasets obtained using XERT at the Australian National Beamline Facility (ANBF), Tsukuba, Japan, are compared with models of Ni-doped borate-glass. This high-accuracy of XERT gives better opportunity for accurate comparison of potentially more accurate ab. initio models. Structures start with a simple NiO₆ Octahedral structure, augmented with adjacent tetragonal sites, occupied either with boron or lithium atoms.

With this improved methodology, X-ray absorption fine structure (XAFS) is compared with models using Demeter and ifeffit, together with software extensions developed within our group, such as ifeffit-like and non-linear-iterpolative-mu2chi. This presentation includes the steps taken to calculate models with increasing accuracy, using both Demeter and ifeffit in a trend study (See Figure) and a loop-process. These programs, each with their own strengths, are used in composite to improve structures, driven and guided by decreasing output parameters such as χ^2_{reduced} . A useful structure is finally obtained via a trend study whereby fitted motifs of borate and lithium-oxide are added to the Ni-O₆ Octahedral to find whether boron or lithium is in higher proportion at tetragonal sites close to Ni. This simple methodology is strong enough to give definitive results. Pitfalls and interesting nuances associated with this loop-process will be discussed.

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Keywords: [Ni-doped borate](#), [glass](#), [XAFS](#)