Crystal Chemistry of Boron-Containing Minerals by Single-Crystal Neutron Diffraction

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Many natural and highly stable minerals contain a significantly high amount of boron which makes their synthetic counterparts of interest as potential neutron absorbers or hosts for storage of nuclear waste. Examples include londonite, with ideal formula $(Cs,K)Al_4Be_4(B,Be)_{12}O_{28}$, and hambergite, with formula $Be_2BO_3(OH)_{0.96}F_{0.04}$. Single-crystal neutron diffraction is well suited to determining the B/Be distribution and the presence or location of H atoms in these minerals but the high neutron attenuation of B requires very short neutron wavelengths and/or crystal volumes that are considerably smaller than those traditionally desired for neutron diffraction. Here we describe the principal novel neutron diffraction techniques that we used to determine the complete crystal structures of londonite [1] and hambergite [2].

For londonite, neutron Laue diffraction on OrientExpress at the Institut Laue-Langevin (ILL), Grenoble, was an efficient way to select a good quality small crystal for further study on the monochromatic diffractometer D9, also at the ILL, at the short wavelength of 0.7058 Å from the hot neutron source. For hambergite, neutron Laue diffraction using KOALA [3] at the OPAL reactor at ANSTO, yielded excellent diffraction data within 36 hours from two small crystals, 2 mm^3 in volume.

[1] G.D. Gatta, P. Vignola, G.J. McIntyre and V. Diella, Am. Miner. 95, 1467 (2010).
[2] G.D. Gatta, G.J. McIntyre, G. Bromiley, A. Guastoni and F. Nestola, Am. Miner. In press (2012).
[3] N. Sharma, T. Söhnel, G.J. McIntyre, R. Piltz and C.D. Ling, J. Phys.: Conf. Ser. 251, 012028 (2010)