

Determining Pb/Bi Distributions using High-Energy Resonant Scattering at K Edges

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Powder diffraction data collected at just below both the Pb and Bi K edges (88.005 keV and 90.526 keV respectively), and ~86 keV on an imaging plate detector have been used to examine the Pb/Bi distribution over the 11 crystallographically distinct sites in $\text{Pb}_5\text{Bi}_6\text{Se}_{14}$. Specialized x-ray optics with excellent energy resolution and stability were used for the experiment. Even with the relatively low scattering contrast that is available at the K edges, it was possible to determine the Pb/Bi distribution and probe the presence of cation site vacancies in the material. The current results indicated that resonant scattering measurements at high-energy K edges are a viable, and perhaps preferable, route to site occupancies when neutrons provide insufficient contrast and absorption from the sample or sample environment/container is a major barrier to the acquisition of high-quality resonant scattering data at lower energy edges.

Use of the Advance Photon Source was supported by the U.S. Department of Energy, Office of Sciences, Office of Basic Energy Sciences, under Contract No. W-31-109-Eng-38.

Keywords: synchrotron powder diffraction, anomalous scattering method, high-energy x-ray diffraction