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High-energy Resonant Scattering Studies of the Pb/Bi Distribution in the Thermoelectric Material $Pb_5Bi_6Se_{14}$. Yuegang Zhang[1], Sarvjit D. Shastri[1], Deming Shu[1], Peter L. Lee[1], Duck-Young Chung[2], Mercouri G. Kanatzidis[2], Angus P. Wilkinson[3], Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, [2]Dept. of Chemistry, Michigan State Univ., East Lansing, MI 48824, [3]School of Chemistry and Biochemistry, Georgia Inst. of Technology, Atlanta, GA 30332.

$Pb_5Bi_6Se_{14}$ was prepared because of its potential for enhanced thermoelectric properties. The Pb and Bi atoms are distributed over eleven crystallographically distinct sites in this compound. Resonant scattering measurements employing the Pb and Bi K edges, at ~ 90 keV, get around the absorption problem. The recently developed high-resolution high-energy x-ray optics at the 1-ID beam line of the Advanced Photon Source achieve a narrow energy bandwidth (~6eV at 90 keV) and excellent energy stability. Rietveld refinement using the GSAS program with combined data sets gave convincing Pb/Bi occupancy values. This experiment demonstrates that very high energy resonant scattering can be a useful tool for site occupancy determinations in complex materials.

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