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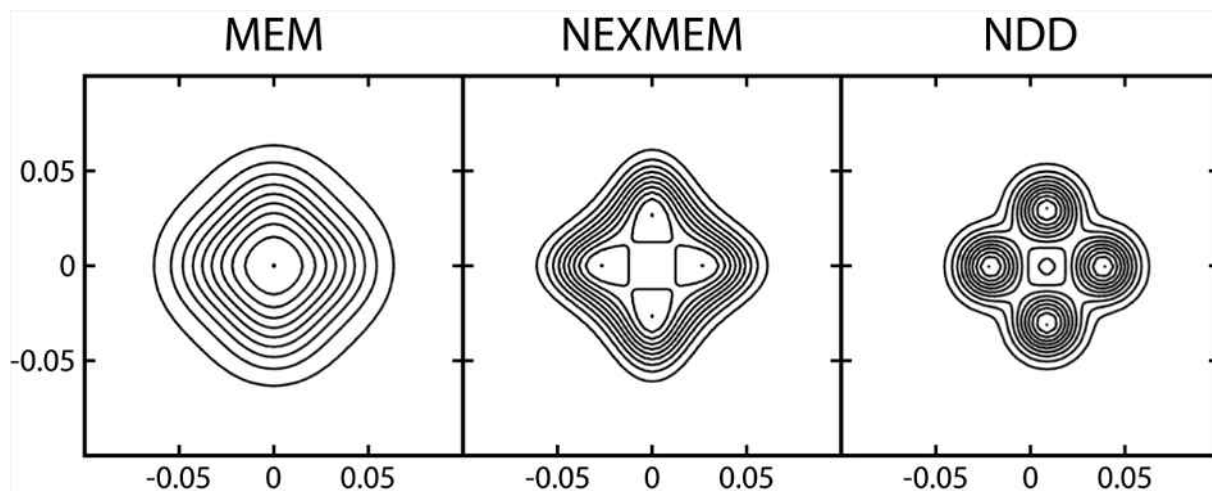
Nuclear Enhanced MEM Used to Analyze Local Distortions in Lead Chalcogenides

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We introduce a novel method for reconstructing nuclear density distributions (NDDs): Nuclear Enhanced X-ray Maximum Entropy Method (NEXMEM). NEXMEM offers an alternative route to experimental NDDs, exploiting the superior quality of synchrotron X-ray data compared to neutron data. The method was conceived to analyse local distortions in the thermoelectric lead chalcogenides, PbX (X = S, Se, Te). Thermoelectric materials are functional materials with the unique ability to interconvert heat and electricity, holding much promise for green energy solutions such as waste heat recovery. The extraordinary thermoelectric performance of binary lead chalcogenides has caused huge research activity, but the mechanisms governing their unexpected low thermal conductivity still remain a controversial topic. It has been proposed to result from giant anharmonic phonon scattering or from local fluctuating dipoles on the Pb site.[1,2] No macroscopic symmetry change are associated with these effects, rendering them invisible to conventional crystallographic techniques. For this reason PbX was until recently believed to adopt the ideal, undistorted rock-salt structure. In the present study, we investigate PbX using multi-temperature synchrotron powder X-ray diffraction data in combination with the maximum entropy method (MEM) and NEXMEM. In addition NEXMEM has been validated by testing against simulated powder diffraction data of PbTe with known displacements of Pb. The increased resolution of NEXMEM proved essential for resolving Pb-displacement of 0.2 Å in simulated data. The figure below shows Pb in the (100) plane for MEM, NEXMEM and the actual NDD of the test structure. Our findings outline the extent of disorder in lead chalcogenides, promoting our understanding of this class of high-performance thermoelectric materials. Furthermore we introduce NEXMEM which can be used for widespread characterization of subtle atomic features in crystals with unusual properties.

[1] E. S. Bozin et al., *Science*, 2010, 330, 1660-1663, [2] O. Delaire et al., *Nature Materials*, 2011, 10, 614-619



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