Nuclear-weighted X-ray maximum entropy method – NXMEM

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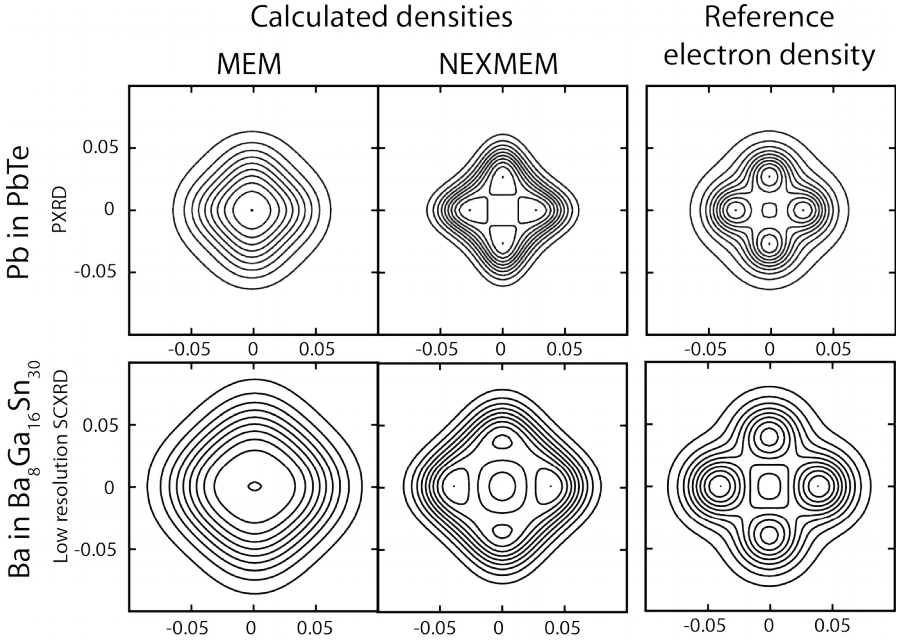
Subtle structural features such as disorder and anharmonic motion may be accurately characterized from nuclear density distributions (NDDs). As a viable alternative to neutron diffraction, we introduce a new approach named the nuclear-weighted X-ray maximum entropy method (NXMEM) for reconstructing pseudo NDDs. By normalization of structure factors, it calculates an electron-weighted nuclear density distribution (eNDD), exploiting that X-ray diffraction delivers data of superior quality, requires smaller sample volumes and has higher availability.[1] NXMEM is tested on two widely different systems: PbTe and $Ba_8Ga_{16}Sn_{30}$. Both are thermoelectric materials with very low thermal conductivity. The origin of their low thermal conductivity remains a controversial subject. A key to understand such properties is the determination of the atomic distribution of Pb and Ba, which may be disordered over closely spaced symmetry equivalent sites.[2,3]

NXMEM was compared to regular MEM by applying to both simulated and experimental powder (PbTe) and single crystal X-ray diffraction ($Ba_8Ga_{16}Sn_{30}$). The figure below shows 2 examples where NXMEM outperforms the regular MEM by resolving the closely spaced atomic positions and recovers more accurate quantitative information. The relative resolution enhancement correlates with the amount of available data, rendering NXMEM especially powerful for powder and low-resolution single-crystal diffraction. Its ability to handle low-resolution data makes NXMEM attractive for cases where resolution is inherently limited e.g. high pressure studies and nano-crystalline/strained samples.

The NXMEM procedure can be implemented in existing software and facilitates widespread characterization of disorder in functional materials.



[1] S. Christensen et al., Acta Cryst. A, 2015, **71**, 9-19

[2] E. S. Bozin et al., Science, 2010, **330**, 1660-1663

[3] S. Christensen. et al., Dalton Trans., 2013, **42**, 14766.