Enhanced thermoelectric and piezoelectric materials by aberration-corrected STEM

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Aberration-corrected scanning transmission electron microscopy (STEM) can locate atomic columns to picometer precision, allowing new insights into structure-property relations in complex functional materials, which can in turn guide the design of new materials with improved properties. Examples will be presented from two representative functional materials, specifically piezoelectric and thermoelectric materials. Results were obtained with the National University of Singapore's JEOL ARM200F STEM.

Piezoelectric materials translate electrical energy into mechanical strain, and vice versa, finding broad application as electronic and electro-mechanical devices. Most materials in current use contain lead, so the development of suitable lead-free alternatives is urgently required. To enable improved properties a fundamental understanding is required of the actual mechanisms involved at the atomic or unit cell level. It is well known that giant responses occur near structural phase boundaries, but the atomistic understanding of the origin of the response has been lacking. By employing atomic-resolution polarization mapping we can uncover the general structural origin of the giant response, a coexistence of ferroelectric phases inside nanodomains allowing gradual polarization rotation between them in response to the applied field. Combined with systematic density functional calculations, we have significantly enhanced the properties of (K,Na)NbO3 and BaTiO3 based lead-free piezoceramics.[1-3]

Thermoelectric materials translate electrical energy into thermal energy, and vice versa, and hold promise for solid-state refrigeration and harvesting electric power from waste heat. Structural defects have a major influence on thermal and electrical transport properties.[4] Nanostructuring has been widely used to enhance thermoelectric properties, however, atomic-scale defects have been difficult to quantify via traditional methods. The improved sensitivity of aberration-corrected STEM has now allowed the direct observation of intrinsic Pb vacancies and extrinsic Cu interstitials in PbTe thermoelectric, revealing the critical roles of Cu for the simultaneous optimization of phonon and carrier transport.[5] Similar structural origins are proposed for the new-generation "Phonon glass, electron crystal" materials such as SnSe and CoSb3.

References:

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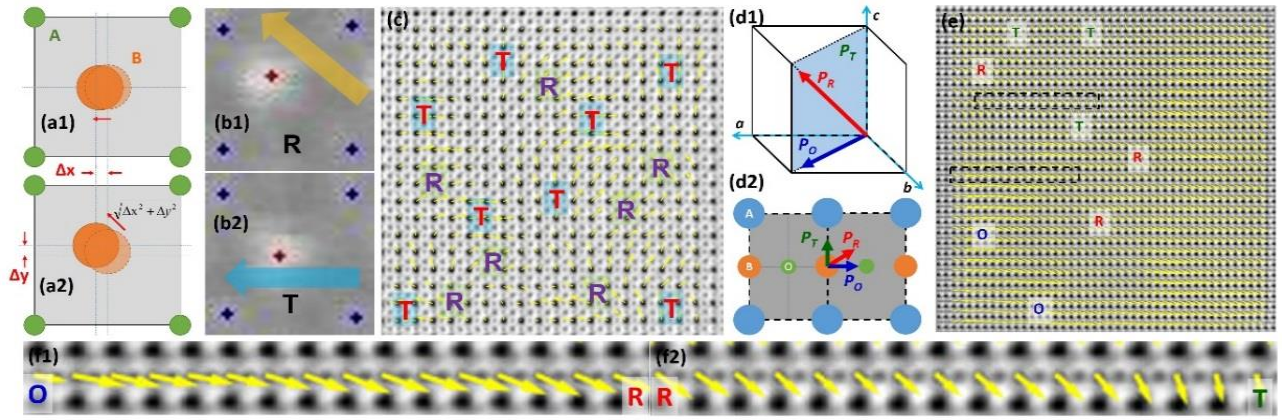

Figure 1. Structural models illustrating phase coexistence (a1,a2) and gradual polarization rotation (d1,d2). (b1,b2) STEM HAADF and (c) ABF images of KNN-based material with polarization map revealing intimate R+T phase coexistence. (e) ABF image of BT-based material with polarization map showing R+T+O phase coexistence. (f1,f2) Schematic showing gradual polarization rotation between R, O, and T phases. Adapted from [2,3].

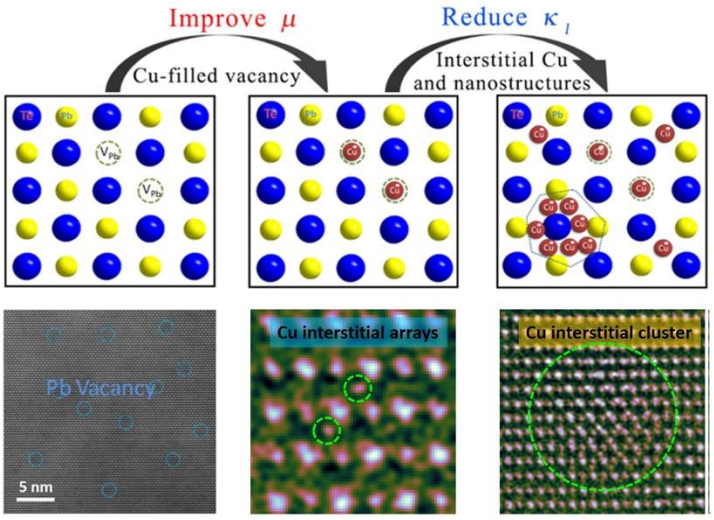

Figure 2. Top: Schematic showing the roles of Cu in PbTe, filling the intrinsic Pb vacancies to enhance carrier mobility and reducing the lattice thermal conductivity through scattering all-wavelength phonons via forming interstitials, clusters and precipitates. Bottom, direct imaging of the defects. Reproduced from [5].

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