Structural origin of high piezoelectricity at phase boundary: nanoscale phase coexistence and gradual polarization rotation

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Piezoelectric materials interconvert electrical energy into mechanical energy, and are widely used for electronic devices. Almost all are toxic lead-based compounds, which are soon to be banned from use in many regions of the world. Hence, there is an urgent need for replacement by lead-free materials. However, so far, lead-free piezoelectrics have not been able to provide competitive performance to the lead-based materials. Key to the academic problem is a lack of fundamental understanding on the actual mechanisms involved at the microscopic (unit cell) level. While it is understood that giant responses occur near structural phase boundaries, there is at present no atomistic understanding of the origin of the response. New materials have therefore been synthesized largely by informed trial and error.

Recently our team has had notable breakthroughs in improving the properties of (K,Na)NbO_3 (KNN) based [1-2] and $BaTiO_3$ (BT) based [3] perovskite ceramics through alloying to engineer the phase boundaries into the desired temperature regime, and simultaneously improving the temperature stability. Electron microscopy has indicated a hierarchical structure of nanodomains with coexisting phases inside, like in the lead-based compounds. Furthermore, precise mapping of atomic displacements reveals a gradual polarization rotation between coexisting phases, as shown in Fig. 1. By directly observing these atomic-scale structural features, we believe we will achieve new understanding of piezoelectric behavior, and as a result be able to synthesize new lead-free materials, bulk and thin film, to eradicate lead-based products from the marketplace, with concomitant environmental and commercial benefits worldwide.

References

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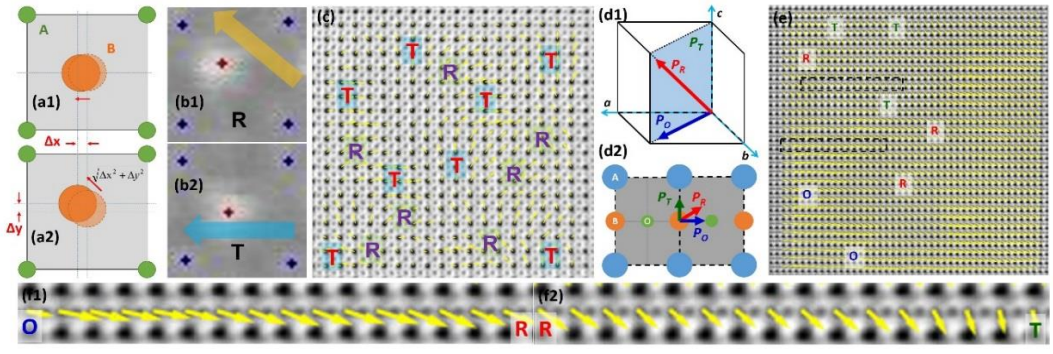

FIG. 1. (a1,a2) and (d1,d2) structural models; (b1,b2) and (c) HAADF and ABF images of KNN-based material with polarization map, R+T; (e) ABF image of BT-based material with polarization map, R+T+O; (f1,f2) Gradual polarization rotation between R, O, and T.