【无机化学论坛】 **Multiscale Structure-Property Relations in High-Performance Piezo-/ferroelectrics of Complex Perovskite Solid Solutions**

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**Multiscale Structure-Property Relations in High-Performance Piezo-/ferroelectrics of Complex Perovskite Solid Solutions**

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 Piezo-/ferroelectric solid solutions of complex perovskite structure, represented by lead zirconate-titanate PbZr1-xTixO3 (PZT) and lead magnesium niobate-lead titanate PbMg1/3Nb2/3O3 – PbTiO3 (PMN-PT), have been the most studied and widely used electroceramic materials for both fundamental research and technological applications as electromechanical sensors and actuators due to their high piezo-/ferroelectric performance. However, their mesoscopic domain structures, local crystal structures and morphotropic phase boundary (MPB) phase symmetry and components remain poorly understood. In order to unveil the origin of high piezo-/ferroelectricity, it is of particular interest to study the single crystals of the canonical piezo-/ferroelectric PZT, which are not only needed for a thorough characterization of the anisotropic properties of this prototype ferroelectric solid solution system, but are also expected to exhibit superior piezo-/ferroelectric performance over the PZT ceramics, and a higher depoling temperature (*T*d) and a higher coercive field (*E*c) than the relaxor-based PMN-PT single crystals, suitable for a broader range of advanced applications.

 Recently, thanks to our capability in growing PZT single crystals with a wide composition range across the MPB and the availability of multiscale characterization and analytical techniques, such as polarized light microscopy, piezoresponse force microscopy (PFM), spherical aberration-corrected transmission electron microscopy, high-resolution neutron total scattering and diffuse scattering, and pair-distribution function analysis, we have gained new insights into the complex local structure, atomic scale polarization rotation, nano-scale domain structure, intricate phase transition and critical behaviour, and tri-critical points in PZT. For instance, the atomic structure of PZT crystals is imaged by means of high-resolution TEM. The accurate Pb displacements and their directions are successfully determined relative to the centre of the four B-cations, on the monoclinic mirror plane. The orientation and distribution of local polarizations indicate a mixture of rhombohedral, tetragonal and monoclinic local symmetry, providing the atomistic evidence for the origin of the monoclinic phase in the PZT of MPB compositions. By synchrotron X-ray diffraction, the structural and domain-wall-motion effects in PZT single crystals are measured and the intrinsic and extrinsic contributions to the piezoelectricity are evaluated quantitatively.

 This series of work provides a better understanding of the relationship between micro-/nano-scopic structure and macroscopic functional properties for the piezo-/ferroelectric materials and for complex perovskite solid solutions in general.