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Keywords: crystals, defects, symmetry

KN-10

The Crystallography of Piezoelectric Perovskites: Domains, Disorder and Disagreements.

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Piezoelectric materials are of enormous importance for a wide range of technological applications from medical imaging to energy harvesting. The industry leader is currently the well-known perovskite solid-solution lead zirconate titanate, PbTixZr1-xO3 (PZT). However, environmental legislation dictates that technological materials should become lead-free in the coming decade – hence, there is an urgent need to find alternatives. To date, the majority of studies have focused on other perovskite solid solutions such as sodium bismuth titanate ($Na_{0.5}Bi_{0.5}TiO_3$, NBT[1]) complexed with barium titanate ($BaTiO_3$, BT) to form NBT-BT or potassium niobate ($KNbO_3$, KN) complexed with sodium niobate ($NaNbO_3$) to form KNN [2]. In making these solid solutions, researchers in lead-free materials are seeking to replicate a key feature of PZT, namely that the phase diagram possesses a special transition region at x=0.48 near to which the piezoelectric properties are massively enhanced. The boundary, which is nearly temperature independent (a technologically advantageous feature) marks a rather abrupt change in the long-range crystal structure, and is termed a morphotropic phase boundary (MPB) after Jaffe *et al* [3] in 1955. For many years, it was understood that this transition was from rhombohedral (R) symmetry on the Zr-rich side to tetragonal (T) symmetry on the right-hand side. The work of Noheda *et al* [4] invoked the presence of an interim monoclinic phase, which appeared neatly to resolve the questions around how a transition from space group *R3m* to *P4mm* could take place smoothly *via* an interim *Cm* subgroup. However, controversy continued, with some accepting the existence of the *Cm* phase, others still supposing a coexistence of *R* and *T* phases, but expressed as nanoscale domains visible only in TEM studies (the so-called adaptive phases model). Still others questioned the whole notion of an MPB at all, postulating that the local scale symmetry of the material was always monoclinic right across the phase diagram so that at on this length-scale, there was not a boundary at all.
In this lecture, I will review the controversies surrounding the study of this (apparently unique) phase boundary in PZT in the context of the last decade of research on lead-free alternatives materials, including our own work on members of the NBT and KNN families. Using the results of combined techniques to look at local structure (NMR and x-ray diffuse scattering), domain structure (optical and electron microscopies, high-resolution diffraction) and crystal structure (x-ray and neutron diffraction), I will discuss to what extent the properties of PZT have been successfully replicated in lead free materials to date and look at the role of the "MPB" in producing large piezoelectric effects – must we have it or can we manage without?

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KN-11

Structural studies of influenza polymerase: implications for the mechanism of cap-snatching, host adaption and anti-viral drug design.

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Influenza virus polymerase transcribes and replicates the viral RNA genome within the context of a ribonucleoprotein complex that has been hitherto remarkably intractable to high resolution structural analysis. As a result many aspects of the detailed mechanism of action of the polymerase remain obscure, despite years of study. However in the last two years, crystal structures of independent domains covering roughly half of the heterotrimeric polymerase have been determined (1). These results will be reviewed with a particular focus on the mRNA cap-binding (2) and endonuclease domains (3), critical for the unique cap-snatching mechanism of influenza viral mRNA transcription. Implications for influenza polymerase assembly (4,5), transcription and host adaptation (5,6) will be discussed as well as the new impetus given to structure-based anti-influenza drug design targeting the polymerase. Finally, structural data will also be presented on the endonuclease domain of another family of cap-snatching viruses, the bunyaviruses.

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