OC57

LATTICE DYNAMICS AND POLAR DOMAIN STRUCTURE OF GIANT-REFRACTION $K_{0.997}Li_{0.003}Ta_{0.64}Nb_{0.36}O_3$ SOLID SOLUTION

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Ferroelectricity in ABO_3 perovskites is generally attributed to off-center displacement of B ions with respect to their coordination environment, eventually clustering into coherently polarized nanoregions (PNR) below the Curie point T_C [1,2]. Although this mechanism has been supported for decades by indirect experimental evidence, to this day little is known about the local structure of the PNR, as well as their relative arrangement at the micrometer scale. In this work, we investigate ferroelectricity in a Li-doped perovskite solid solution $K_{0.997}Li_{0.003}Ta_{0.64}Nb_{0.36}O_3$ (KLTN) displaying giant broadband refraction (n>25) below T_C, where a supercrystal with large-scale periodicity (~5 µm) is observed [3], as illustrated in Fig. 1. Density functional theory calculations performed on the parent structures - ferroelectric $KNbO_3$ and paraelectric $KTaO_3$ – help to rationalize the interplay between Li, Ta and Nb displacements observed in the solid solution through X-ray diffraction (XRD) measurements. In parallel, molecular dynamics simulations calibrated on the same XRD data investigate the atomic structure at higher length scales (~10-100 nm), where the PNR emerge. Observations from *ab-initio* and classical simulations are then combined in order to interpret the temperature-dependent lattice dynamics of KLTN, leading from the room-temperature paraelectric phase to the below-T_c ferroelectric phase. These results provide a basis to rationalize the structural origin of the remarkable optical properties of KLTN.

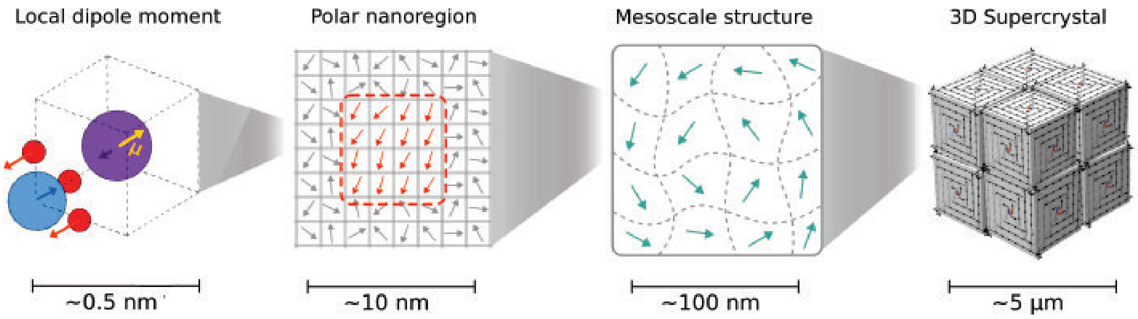

Figure 1. Illustration of the plausible structure of the KLTN solid solution below the Curie point, at different length scales.

[1] V. Polinger et al. Phys. Rev. B 98 (2018) 214102.
[2] M. S. Mark et al. Phys. Rev. Lett. 116 (2016) 207602.
[3] L. Lo Presti et al. Phys. Rev. B 102 (2020) 214110.

Return to List of Contributions