Domain formation and planar defects in NASICON electrolyte materials

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We present results of the internal structure of individual nanocrystalline grains of a range of NASICON ion-conductor materials using Bragg Coherent Diffraction Imaging (BCDI). The samples, prepared by solid state synthesis, are potential solid-state electrolyte materials with high ion conductivities. BCDI is an X-ray imaging method inherently sensitive to strain that takes advantage of the high coherence of the X-ray beams at the latest synchrotron sources. It works by inverting the fine-structured diffraction surrounding the Bragg peaks from individual grains in a powder sample [1]. Images, obtained at the P10 beamline of PETRA-III in Hamburg, reveal a distinct pattern of sub-domains within the grains of most of the samples examined. Figure (a) shows the external shape of one of the grains, measured at the 113 Bragg peak of a $Li_3Ca_{0.5}Ti_{0.5}Zn_{0.5}Sn_{0.5}(PO_4)_3$ crystal The domains, see in cross section in (b), representing an extreme degree of strain, are blocks of crystal phase shifted relative to each other. This indicates the presence of rigid shifts within the crystal lattice and hence the formation of planar crystal defects between them. It is likely that the presence of such defects, not previously identified, could significantly affect the ion transport properties of the materials. We consider how these might originate from the ball-milling steps used to mix the precursor materials used in their solid-state synthesis.

[1] I. Robinson and R. Harder, Nature Materials 8 291-298 (2009)