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Diffuse X-ray Scattering: Probing the Nano-scale Disorder in the Lead-Free Piezoelectric Na_{0.5}Bi_{0.5}TiO₃

Understanding the relationship between the properties of piezoelectrics and its atomic structure is important in enhancing their properties. With the addition of enforced legislations motivating the removal of lead in all electronic products, research into the fundamental properties of lead-free piezoelectric materials is vital.

A promising lead-free piezoelectric is Na0.5Bi0.5TiO3 (NBT), however it is a highly complex perovskite material and the room temperature structure is still debated. The use of conventional scattering methods to analyze Bragg peaks gives information on the long-range average structure that permeates throughout the whole material, and hence it can be difficult to extract information on deviations away this average structure, i.e. the disorder. Scattering that originates from this disorder is known as diffuse scattering. Here, diffuse X-ray synchrotron scattering was employed to deduce the short- to medium-range structures that diverge away from the long-range structure. Analysis of the diffuse scattering has revealed a diverse range of disorder occurring in NBT, which includes octahedral stacking faults, A-site size effects and structural modulations on the order of 10 unit cells. Preliminary modelling of the A-site occupancy has been carried out and modelling of the remaining disordered structures is currently being performed.

By understanding the nano-scale atomic mechanisms that contribute to the electromechanical properties in NBT, we will be closer to exploiting and controlling such properties in future functional materials to allow them to replace current lead technologies.

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