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Investigation of phonon dynamic in single crystal lead-halide perovskites by inelastic neutron scattering

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The lead halide perovskite materials have recently risen to prominence for remarkably high photovoltaic efficiencies in polycrystalline materials that are highly defected [1] Some of the reasons for this good defect tolerance are the very low exciton binding energy and consequent highly delocalized electrons and holes leading to high mobilities in these materials, coupled to low thermal conductance. Other recent work by our group has shown long lifetimes for hot carriers in a range of perovskites with organic lead iodide perovskites having the longest lifetimes [2]. In order to explain those rather promising physical properties, a closer investigation of phonon dynamics is needed. Although ab initio simulations (DFT) can predict phonon dispersions to a reasonably accurate extent (comparison between different phonon modes) [2, 3], scaling their energies to actual phonon energies (particularly at high momenta near the zone edge) can be rather inaccurate. In order to obtain a detailed phonon dispersion to overcome the limits of the ab initio methods, inelastic neutron scattering techniques can be used (as they offer full Brillouin zone mapping and are suitable for large single crystal samples).

The thermal triple axis spectrometer (TAS) on TAIPAN at OPAL reactor at ANSTO was used with the aim to map phonon dispersion of single crystal Methyl Ammonium Lead Halide Perovskites, CH3NH3PbBr3 and CH3NH3PbI3 [4]. The alignment was performed so that we could scan through [h k l] and [0 k l] planes in reciprocal space for MAPbBr3 and MAPbI3 samples, respectively. Assuming the cubic space group, ABX3, for the MAPbBr3 sample, we were able to perform transverse and longitudinal scans along each high symmetry direction in the Brillouin zone (Γ-X and Γ-M) which would ensure the mapping of all phonon modes in the h k plane of the Brillouin zone.

The full phonon dispersions that will be obtained with this method can be of great significance as by adding up to the already simulated data we will be able to have a deeper insight into the undergoing physics that is responsible for the previously observed properties (such as significantly extended hot carrier lifetimes) where phonon dynamics will play a significant role.

Topic

Advanced Materials

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