In situ imaging of ferroelastic domain dynamics in CsPbBr₃ perovskite nanowires by nanofocused scanning X-ray diffraction

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Metal halide perovskites (MHPs) has shown impressive results in solar cells, light emitting devices, and scintillator applications, but its complex crystal structure is only partially understood and many open questions are still to be answered [1]. In particular, a method to image the dynamics of the nanoscale ferroelastic domains in MHPs requires a challenging combination of high spatial resolution and long penetration depth. With the recent development in X-ray optics it is now possible to focus X-rays down to the nanoscale. Combining the traditional high sensitivity to lattice spacing and tilt, as well as its characteristic to probe deep into the sample, nanofocused scanning X-ray diffraction is a unique powerful technique on the study of MHPs domain dynamics [2].

In this work, we demonstrate in situ temperature-dependent imaging of ferroelastic domains in a single nanowire of metal halide perovskite, CsPbBr₃, using scanning X-ray diffraction with a 60 nm beam [3] to retrieve local structural properties for temperatures up to 140 °C [4]. We observed a single Bragg peak at room temperature, but at 80 °C, four new Bragg peaks appeared, originating in different real-space domains, as depicted in Fig. 1 (left panels). The originally random domains were arranged in periodic stripes in the center and with a hatched pattern close to the edges, as one can see in Fig. 1 (right panels). Reciprocal space mapping at 80 °C was used to quantify the local strain and lattice tilts, revealing the ferroelastic nature of the domains. The domains display a partial stability to further temperature changes. Our results show the dynamics of nanoscale ferroelastic domain formation within a single-crystal perovskite nanostructure, which is important both for the fundamental understanding of these materials and for the development of perovskite-based devices.

**Figure 1.** Diffraction peaks and the corresponding scanning X-ray diffraction nanowire map at 30 °C (top panels) and 80 °C (bottom panels).

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**Keywords:** perovskite; CsPbBr₃; nanowire; ferroelasticity; X-ray diffraction

This project has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No. 801847). This research was also funded by the Olle Engkvist foundation, NanoLund, and Marie Skłodowska Curie Actions Cofund, Project INCA 600398.

*Acta Cryst.* (2021), A77, C134