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TEM Characterization of the Edges of $CsPb_2Br_5$ Perovskite Crystals

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Edges of $CsPb_2Br_5$ microplates have been characterized by low dose transmission electron microscopy together with energy dispersive spectroscopy measurements. $CsPb_2Br_5$ is a water resistant perovskite similar in character to $CsPbBr_3$ but with a two dimensional Pb-Br framework separated by Cs layers. These two compounds can coexist at the nanoscale forming nanocomposites or core shell arrangements that give rise to stable photoluminescence (PL). Nevertheless the PL properties of the CsPb2Br5 have been under controversy, some reports indicate a strong visible PL while others give inherent PL inactivity. In this work, clean $CsPb_2Br_5$ are synthesized through a simple water induced phase transformation from $CsPbBr_3$ to reduce potential chemical contamination. $CsPbBr_3$ powders are first synthesized using a modified method by mixing 0.5 M $Pb(CH_3COO)_2 \cdot 3H_2O$ and 1 M CsBr in 48% HBr solution at room temperature. $CsPb_2Br_5$ can then be synthesized by dropping $CsPbBr_3$ micro-cubes in water (20-50 times more water in mass) at room temperature. Atomically flat $CsPb_2Br_5$ microplatelets are prepared to distinguish edge photoluminescence from body emission and to prove that single crystal $CsPb_2Br_5$ is a two-dimensional wide bandgap semiconductor. Full details of the physical characterization are given elsewhere [1, 2].

Figure 1 shows phase images of a typical edges on the microplatelets at atomic resolution. The phase image is determined from an exit wave reconstruction (EWR) procedure that involves 40 experimental images at different defoci (MacTempass ®). The TEAM 0.5 electron microscope is used to acquire the experimental images at a dose rate of 20 $e^-/Å^2s$. Both images in Fig. 1 show three different areas with distinctive material phases: near the edge the phase $CsPbBr_3$ can be identified (I), the phase $CsPb_2Br_5$ is located at the farther end (III) and into the bulk of the sample and finally a mixture of phases is imaged in the intermediate region (II). The spatial distribution of phases is better appreciated by using a Fourier transform analysis as that shown in Fig. 2. Apparently the region near the surface (I) forms during the synthesis procedure in connection with chemical distribution of the involved elements. The inverse FFT in Fig. 2c shows patches of the $CsPbBr_3$ inside the mixture region (II) and then the phase $CsPb_2Br_5$ becomes predominant in regions relatively far from the surface (III). EDS measurement confirm the chemical differences observed in atomic resolution phase images.

References:

[1] V. G. Hadjiev *et al*, submitted to Physical Review B (2018).
[2] Y. Wang *et al*, to be published.
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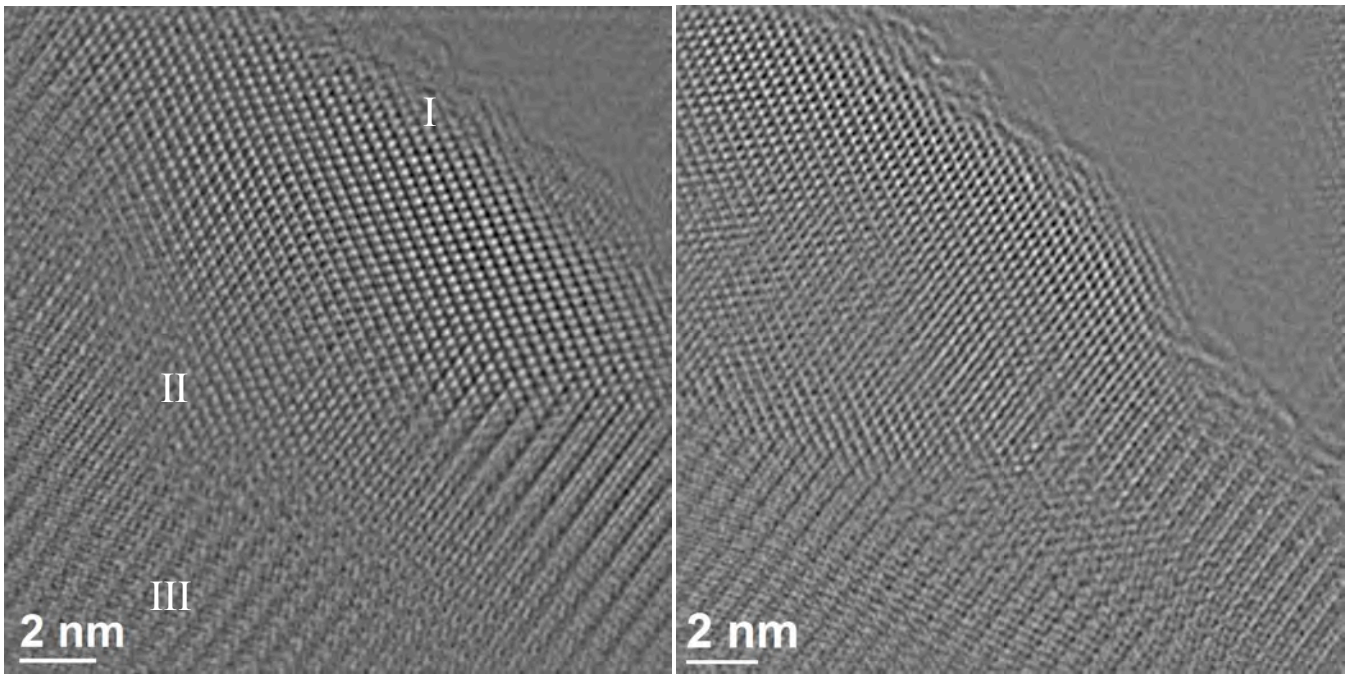

Figure 1. Typical phase images of edges in perovskite microplates. Three different regions are identified as CsPbBr3 (I), a mixture of phases (II) and periodic $CsPb_2Br_5$.

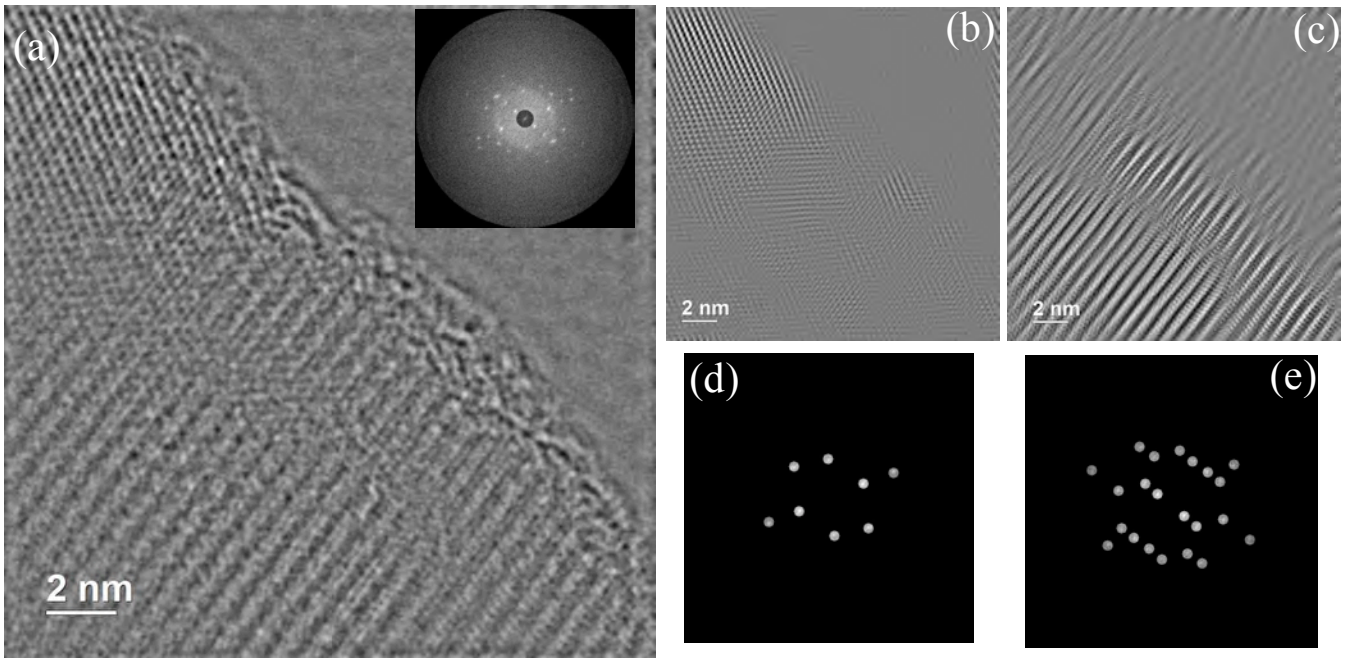

Figure 2. FFT Analysis of phase distribution. (a) Phase image and FFT. (b) IFFT showing distribution of $CsPbBr_3$ phase. (c) IFFT showing distribution of $CsPb_2Br_5$. (d,e) Masks for IFFTs.