Thermal nanoimprint to improve the material properties of $MAPbI_3$

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Perovskites have attracted the interest for a lot of applications in optoelectronics [1] like photo-detectors [2] and solar cells [3] due to their easy preparation by liquid processing. However, the morphology of the material highly depends on the composition of the solution, the solvent and the preparation conditions. As morphology is directly connected with the electrical properties [1] the optimization of the morphology is the primary demand when high-performance devices are addressed. Interestingly, it is reported that the morphology of these perovskite materials can be improved by nanoimprint [2], quite similar to effects observed with the semi-crystalline polymer P3HT [5]. However, a detailed investigation of the processing conditions with nanoimprint that are adequate to improve the properties of e.g. $MAPbI_3$ is still missing.

This investigation starts with defining an adequate treatment temperature for $MAPbI_3$, first. Figure 1a) demonstrates that temperatures up to 200°C may be suitable for imprint. After treatment at higher temperature a distinct color change indicates that the material has decomposed irreversibly. Detailed SEM inspection (Figure 1b,c) shows that degradation has already started at 150°C; the needle-like crystallites represent PbI_2 as a decomposition product. However, under imprint conditions (no air contact), the maximum temperature may be somewhat higher. Figure 2 shows imprinted samples in comparison to a non-imprinted reference. The micrographs clearly indicate that the sample imprinted at 150°C features the best morphology, not only a larger size of the crystals but also no sign of degradation (no needle-like crystals). Figure 3 confirms the optimized morphology with 150°C even when nano-dots were imprinted. With 100°C the crystallites are smaller and wide grain boundaries are still visible. XRD characterization (Figure 4) confirms that degradation took place when the sample was imprinted at 200°C. The improvement of the material by thermal imprint is documented by means of the IV-characteristics of $MAPbI_3$ solar cells. Compared to the pristine device (12.61%) the device after imprint at 150°C features a highly increased efficiency (15.58%). We will report on the details of morphology improvement of $MAPbI_3$ by thermal nanoimprint.

[1] H.S. Jung et al., Small **11**, 10 (2015)
[2] H. Wang et al., ACS Nano **10**, 10921 (2016)
[3] X. Tong et al., Adv. Sci. **3**, 1500201 (2015)
[4] N. Pourdavoud et al., Adv. Mater. 29, 1605003 (2017)
[5] S. Wang et al., J. Vac. Sci. Technol. B **33**, 06F602 (2015)

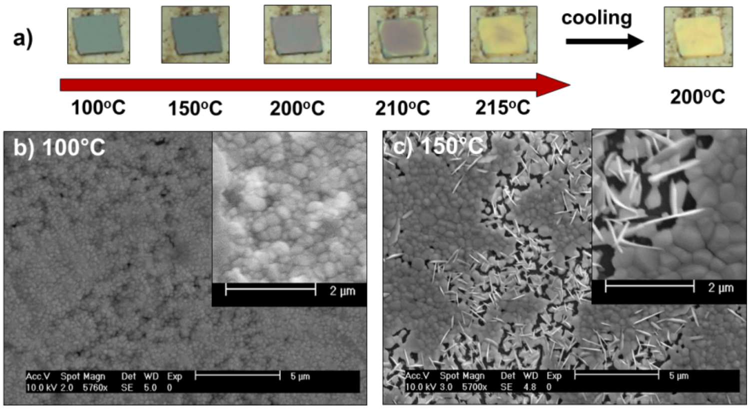

Figure 1: Degradation and morphology change of $MAPbI_3$ during thermal treatment in air. Optical appearance of samples at different temperatures (a) and SEM images after thermal treatment at 100°C (b) and 150°C (c).

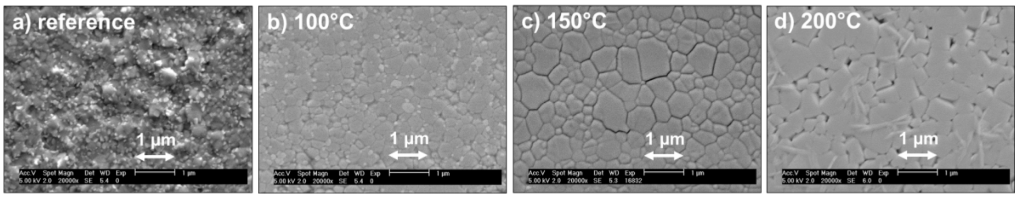

Figure 2: Impact of thermal imprint on morphology. Non-imprinted reference sample (a), samples imprinted with blank Si at 100°C b), 150°C c) and 200°C d).

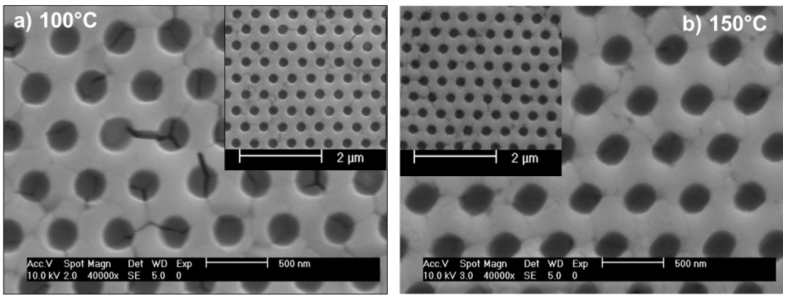

Figure 3: Samples imprinted with pillar structures at 100°C a) and 150°C b).

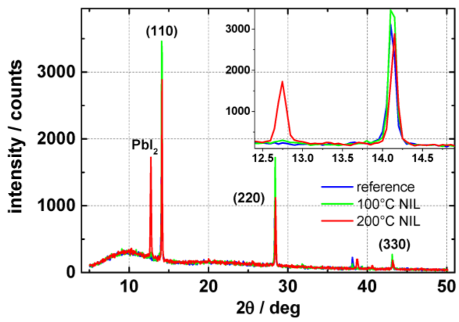

Figure 4: XRD characterization of imprinted sample and pristine reference.

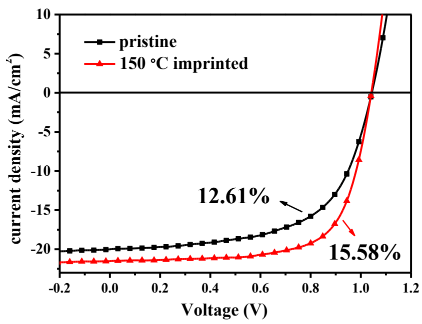

Figure 5: IV-characteristics of solar cells (pristine and imprinted).