Texture of strongly oriented MAPbI3 studied by wide reciprocal-space mapping

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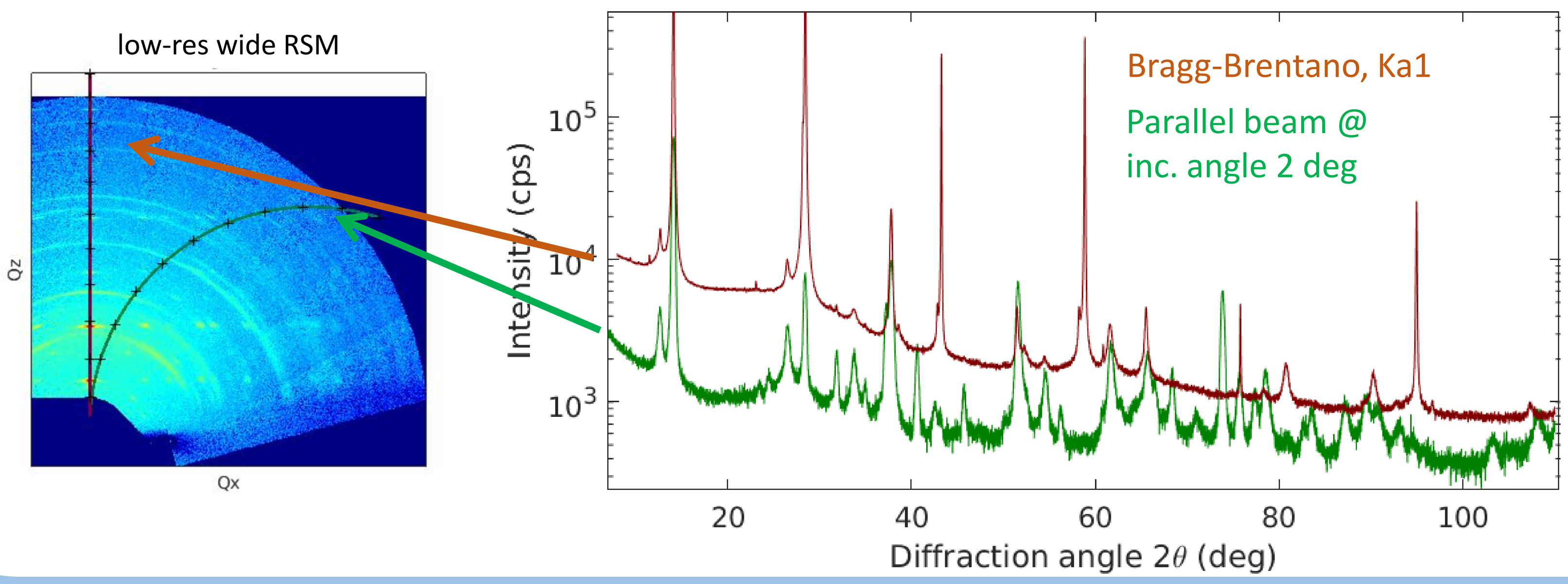
Motivation

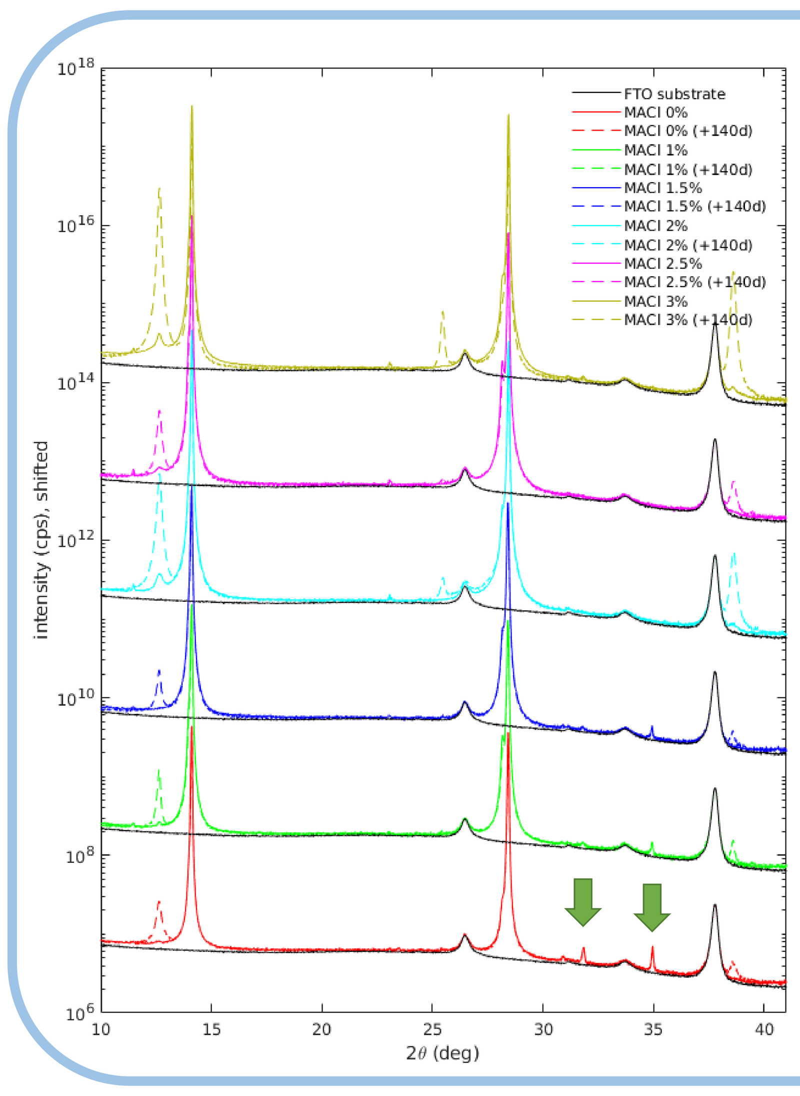
Polycrystalline organic perovskites such as $CH_3NH_3PbI_3$ (MAPbI3) quite often form strongly oriented polycrystalline layers with complex multicomponent fibre texture. Prefererential orientation as well as other microstructure parameters of MAPbI3 layers are strongly affected by the preparation procedure [1] and are correlated with the stability and performance of the final sollar cells. We observed the change in texture composition and the degradation rate for different concentrations of MACl additive (0 % – 3 %) present during the preparation of the MAPBI3 layer preparation.

Method

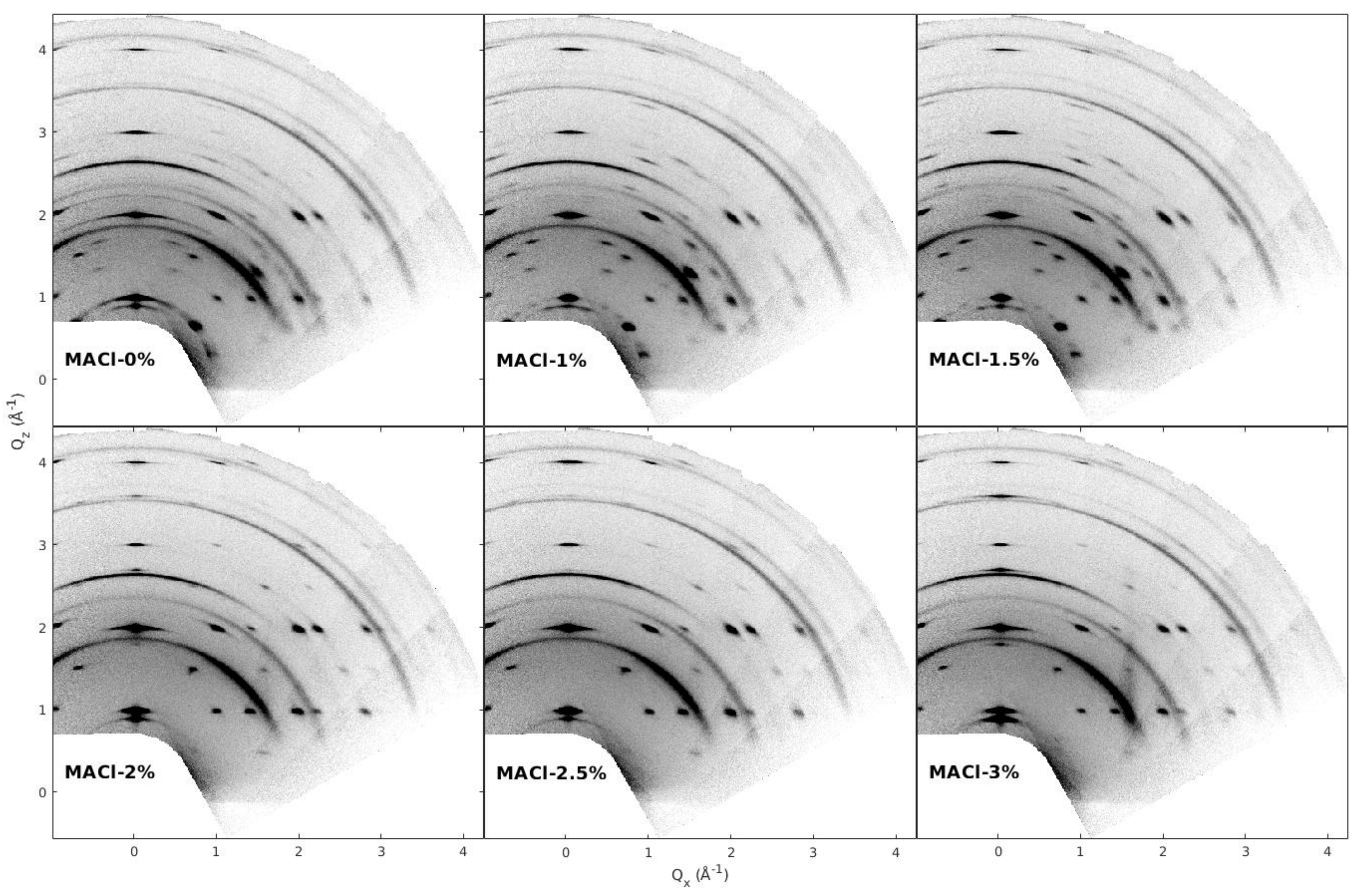
In order to fully determine the texture of the layers, one can use well-established but time consuming pole-figure measurement; however, it is not very optimal for materials with large low-symmetric unit cells. Here the number of observable peaks is high, therefore their diffraction angles are partially overlapping, and further possible strain can induce some peak shift. On the other hand, in this case it is very convenient to use a fast reciprocal space mapping method, which is quite fast and it can be used blindly without prior knowledge of the peak positions because the whole cut of reciprocal space is recorded and analyzed ex post.

As expected for textured layer, BB scan and GID pattern are not very similar due to their different path in reciprocal space.





PXRD patterns (Bragg-Brentano) for MAPbI3 (MACl-assisted preparation) have been collected for different MACl concentrations. Mainly MAPbI3 hh0 peaks are present due to the strong (110) texture. The degradation of the sample over time is manifested by the appearance of PbI2 Bragg reflections, their intensities correlate with MACl concentration. *Quite often people use only these intensities to compare the "crystallinity degree" and stability.* This simplification can lead to data misinterpretation, since the texture which differs for various samples is completely neglected. In our case, **further peaks are also visible for higher MACl concentration**, and at least semi-quantitative texture analysis is necessary.

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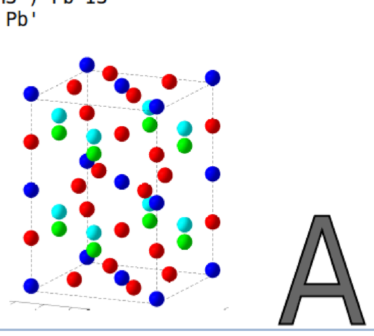


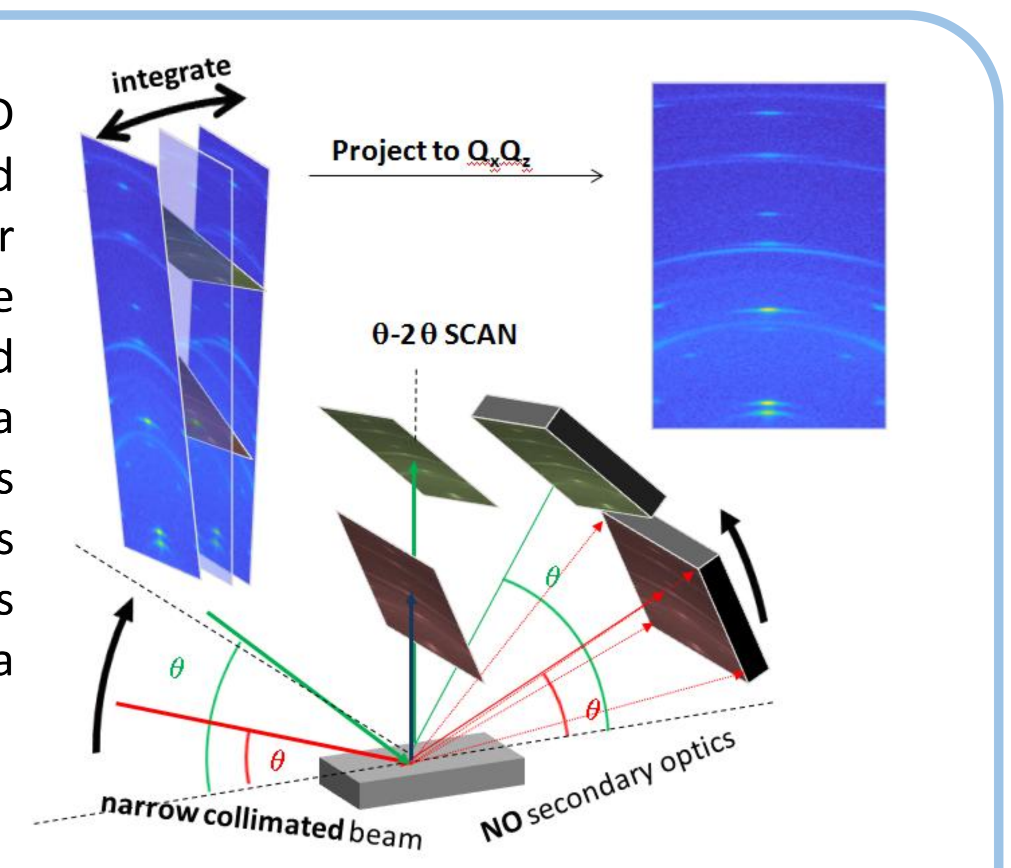
Texture model:

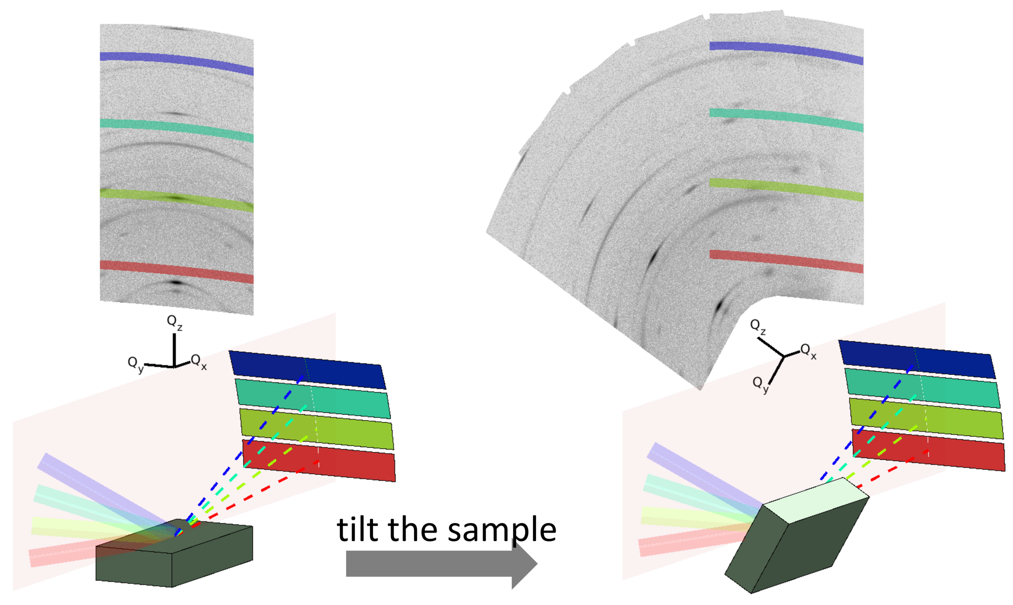
(110) **(021)** **(130)**

parallel to the surface

Experimental

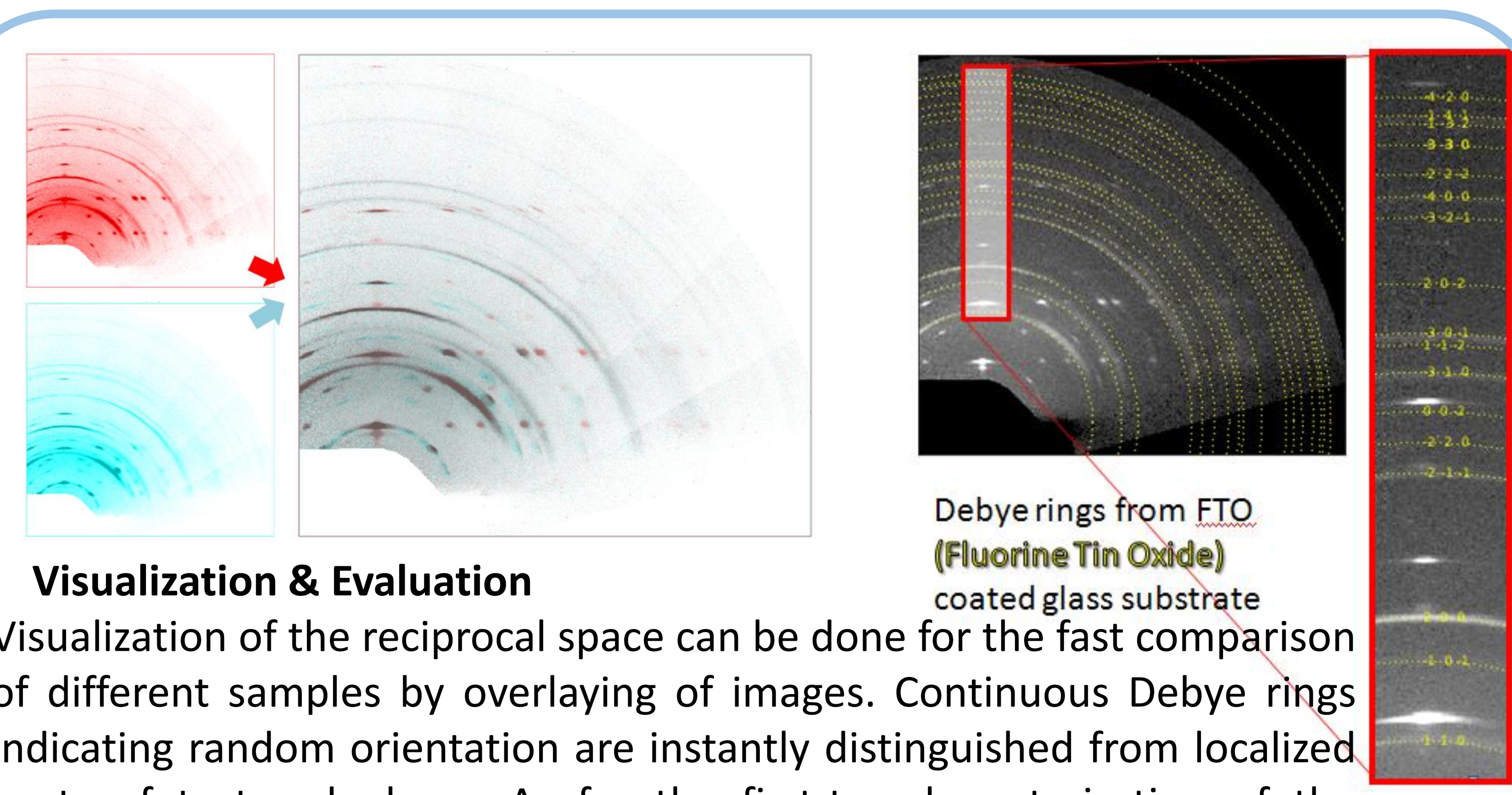
To speed up the measurement, 2D detector is placed closely behind the sample. Using the shorter sample-detector distance, the resolution is partially sacrificed while the reciprocal space area observed by the detector is dramatically extended. In this configuration, the continuous theta-2theta scan fully probes a long stripe in a reciprocal space.





By measuring several such stripes for different sample tilts, it is easy to reveal the full planar cut of the reciprocal space, and surprisingly the total acquisition time can be only tens of minutes for strongly oriented layers.

Moreover, such measurement can be performed for different sample azimuth in order to obtain different planar cuts. This is desirable for single-crystal substrates, for which the surface symmetry can be followed.

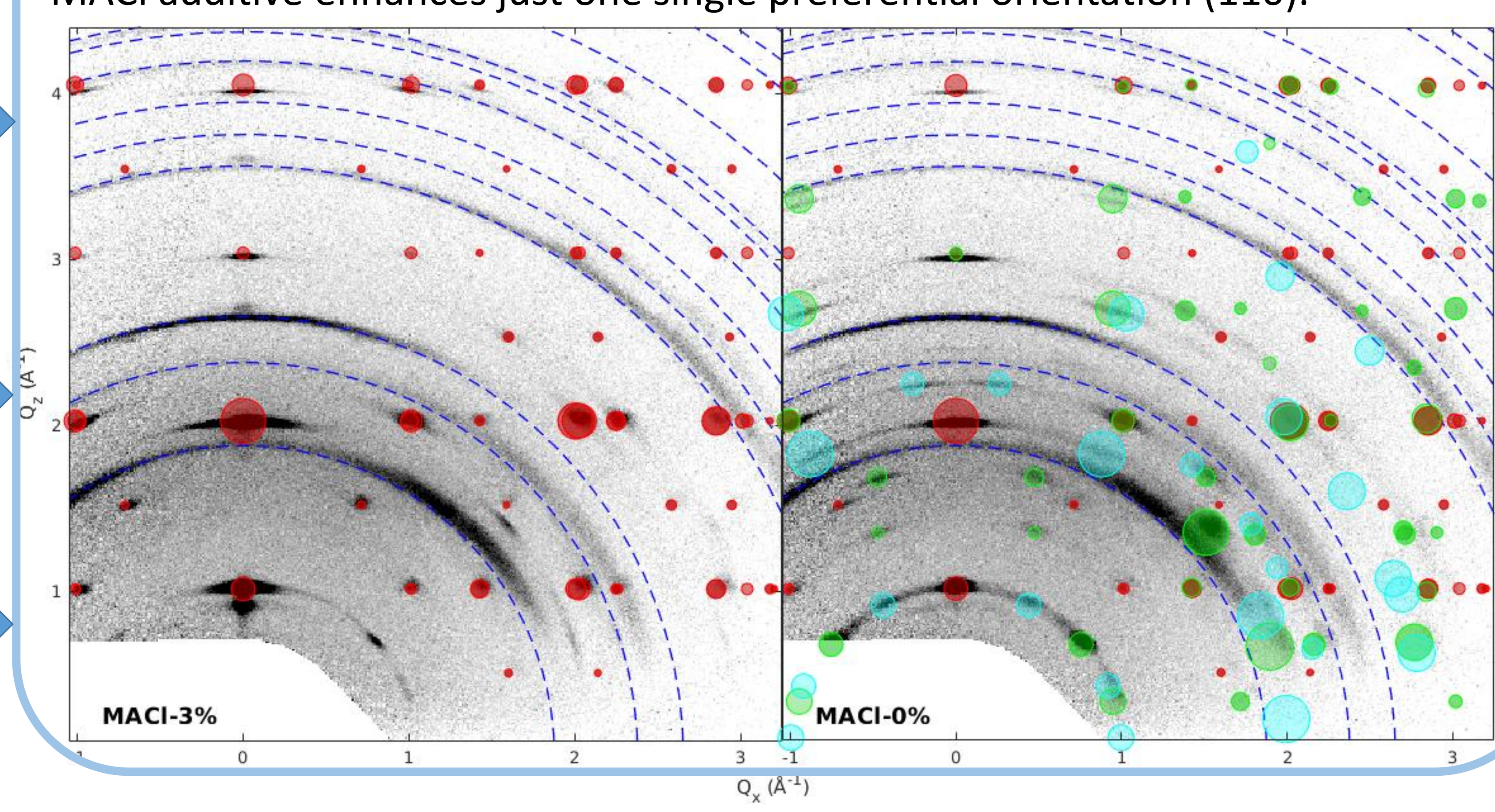


Visualization & Evaluation

Visualization of the reciprocal space can be done for the fast comparison of different samples by overlaying of images. Continuous Debye rings indicating random orientation are instantly distinguished from localized spots of textured phase. As for the first-try characterization of the samples, obtained images are compared with the simulations based on some expected phase/texture model giving semi-quantitative results.

Results

A low concentration of MACl additive results in a multi-component texture. The strongest (110) major component is accompanied by medium-populated (021) component and weak (130) component. On the contrary, a high concentration MACl additive enhances just one single preferential orientation (110).



Literature: [1] Amalathas et al, *ACS Appl. Energy Mater.* 2020, 3, 12484−12493

Acknowledgement

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