Interface Crystallography of a Growing Interface: KDP $\{101\}$ and $\{100\}$

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In crystal growth from solution, the solvent is often found to determine the morphology of the crystal or the particular polymorph that is formed. Using in situ X-ray diffraction it is possible to determine the atomic-scale structure at a solid-liquid interface [1], and thus one can try to determine the microscopic origin of the solvent effect.

Here we present our results on the solid-liquid interface structure of the $\{101\}$ and $\{100\}$ faces of KDP (KH₂PO₄) in aqueous growth solutions as a function of the solution pH. The morphology of KDP crystals changes as a function of the pH, the largest effect coming from a decrease in growth velocity of the $\{101\}$ face for non-stoichiometric conditions. Using the high-intensity X-ray beams from the ESRF synchrotron, we find remarkably large changes in the liquid ordering as a function of pH for the $\{101\}$ face, while the $\{100\}$ face is largely unchanged. For high pH, we observe crystalline preordering of K-ions in the solution at the $\{101\}$ face.

The KDP{101} face terminates in a positive K-layer, but our results indicate that an electrochemical interpretation of the interface is less correct than a crystallographic point of view.

[1] Vlieg E., Surf. Sci., 2002, 500, 458

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