



	Experiment title: Influence of pH on interface structure of KDP	Experiment number: 26-02-175
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Report: (max. 2 pages)

Crystal growth from a solution is a very important process that is used in laboratories as well as in industry. An innumerable number of organic and inorganic crystals are grown in this fashion. It is clear that in the process of crystal growth, the interface region plays a major role. Small amounts of additives can drastically change the properties of this region and thus modify the surface energy and the morphology of the crystals [1].

In the case of KDP (KH_2PO_4 potassium di-hydrogen phosphate) crystals, we have been able explain the influence of cations on the growth shape by determining the crystallographic structure of the relevant growth faces {100} and {101} [2]. Another way to change the KDP crystal morphology is to change the pH of the growth solution. During normal crystal growth conditions (pH = 4.6) the {101} faces grow fast. When the pH of the solution is changed to a value of about 3, the growth in the {101} directions is much slower. This effect is used in practice to grow big KDP crystals of high quality [3].

The aim of this experiment was to determine the interface structure of KDP in different pH conditions. We used our experimental cell that was designed to do X-ray investigation in a liquid environment. The beam line conditions were excellent, and we were able to acquire data sets consisting of several rods for both faces and for pH values of 3, 4.6 and 5. In most cases the changes in structure factor are small, as expected, since major structural rearrangements seem unlikely for relatively mild changes in the environment. We were pleasantly surprised, therefore, to find a remarkably large difference for the pH = 5 case on the {101} face. The figure shows the difference for the (10), (01), (00) and (20) rods for pH values of 3 and 5.

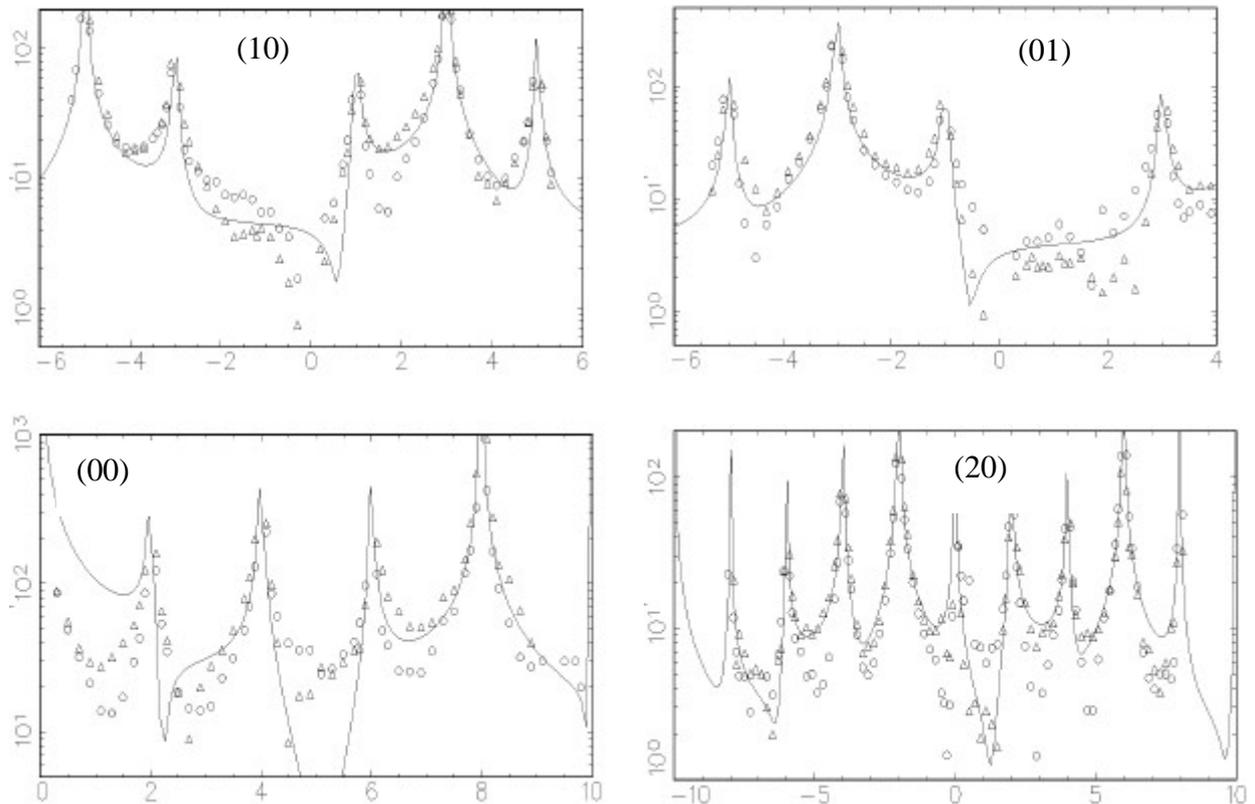


Fig. 1. For different rods as measured on $KDP\{101\}$. Circles represent data for $pH=5$, triangles represent data for $pH=3$. The solid curve is a calculation for K -terminated crystal in which neither relaxation nor liquid structure are taken into account.

The interpretation of these results has to await a full analysis, in which the ordering of the liquid has to be taken into account as well. We will benefit from our earlier work in which the water layer thickness was varied [4]. The new $pH = 4.6$ data is in excellent agreement with these earlier results. At this moment we can only conclude that there is a surprisingly large effect of pH on the interface structure of the $\{101\}$ face. We expect to correlate this with the observed difference in growth morphology of KDP crystals.

References

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4. Reedijk, M.F., et al., *Liquid order at the interface of KDP crystals with water: evidence for icelike layers*. *Phys. Rev. Lett.*, 2003, **90**, 066103.