



	Experiment title: The structure of (R,R) tartaric acid on Cu(110)	Experiment number: SI-883
Beamline: ID3	Date of experiment: from: 07 May 2003 to: 15 May 2003	Date of report: 29.10.2003
Shifts:	Local contact(s): Chris Walker	<i>Received at ESRF:</i>

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Report:

(R,R) tartaric acid (TA) on Cu(110) is a model system for heterogeneous enantioselective catalysis. The TA molecules can adsorb in a variety of phases, of which only one is potentially catalytically active [1]. The aim of this project was to determine the surface structure of TA on Cu(110) for this phase, which is denoted as the (9,0,1,2) phase in matrix notation. In particular, it is of interest to determine whether the TA molecules induce chirality in the Cu(110) substrate, because this could play a role in the enantioselectivity.

We collected data sets for five separate surface preparations, each set consisting of more than 120 non-equivalent reflections. Part of the data is shown in figure 1. The TA overlayer is clearly visible. To our surprise, however, the modulation of the specular rod was different from that observed in an earlier experiment on DUBBLE (exp. 26-02-119). Apparently, we had different surface phases for the two

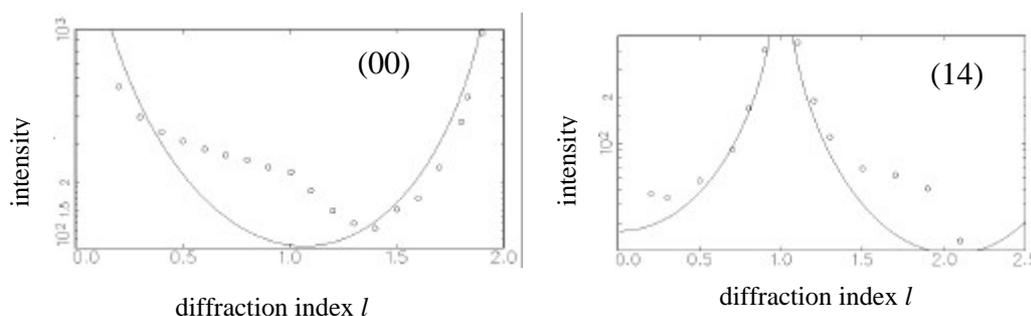


Fig. 1 Two crystal truncation rods measured after deposition of tartaric acid. The solid curves show calculated profiles for a bulk-terminated Cu(110) crystal.

experiments. One of the lessons from these experiments is therefore that it is difficult to make the correct phase in a reproducible manner. While we had prepared the correct (9,0,1,2) phase in our own vacuum system in Nijmegen as determined from RHEED, we did not have electron diffraction available at ID3. We had hoped to do this using X-ray diffraction, but it turned out to be impossible to detect the fractional-order reflections. This is due to two reasons: (1) there are four different surface phases, so many locations in reciprocal space need to be scanned and (2) the long-range order is limited, thus the signal-to-background ratio is low and scanning takes a long time.

We therefore had to limit ourselves to measuring the integer-order rods. These turned out to be surprisingly reproducible for several different surface preparations. We have in the meantime concluded this is due to the fact that, after several depositions, the vacuum chamber contains enough tartaric acid to cover the substrate, even after a cleaning cycle. (The vapour pressure of this organic material is quite high, deposition is done at 90°C). The proof of this was obtained by performing RHEED in Nijmegen on the sample we prepared at the ESRF, see figure 2. The surface phase is stable enough to show a clear RHEED pattern after a moderate anneal, even after a transfer through air! The phase turned out to be the high-coverage (4,1,2,5) phase. Analysis is in progress to fit the integer-order data with an appropriate model. From this we expect to determine the orientation and height of the tartaric acid molecules in this phase, but the lack of fractional-order data will not allow the determination of all the structural details.

In summary, we can clearly detect tartaric acid on Cu(110), but for the preparation of the correct phase with large domains, RHEED (or LEED) is required and pollution of the chamber with tartaric acid needs to be avoided.

[1] M. Ortega Lorenzo, C.J. Baddeley, C. Muryn and R. Raval, Nature 404 (2000) 376.

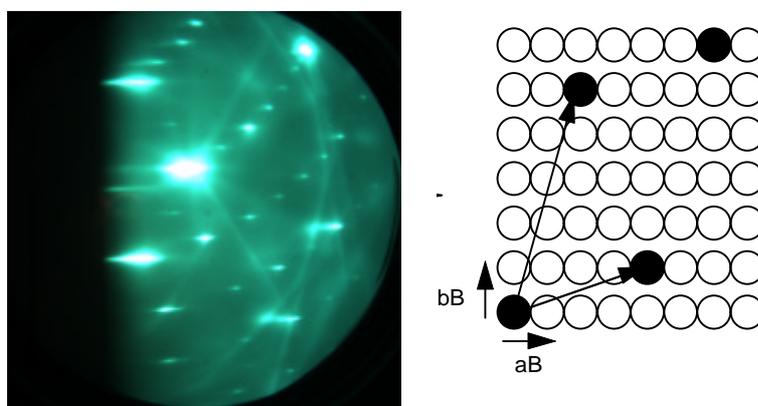


Fig. 2. RHEED pattern and unit cell of the (4,1,2,5) phase of tartaric acid on Cu(110)