ESRF	**Experiment title:** STRUCTURE OF THE DIAMOND (111)/LIQUID-GA INTERFACE	**Experiment number:** SI 87
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Report:

We have studied the ordering phenomena that have been predicted to occur[1] in a liquid that is in contact with a crystalline solid using X-ray diffraction. Near the interface, the liquid is expected to exhibit atomic layering in the direction along the surface normal, as well as ordering parallel to the interracial plane. These theoretical predictions have not been counterparted by experimental verifications that were extended towards Ångstrom resolution. For our model system we have chosen a clean diamond(111) crystal and as a liquid we have used Ga.

The scattering geometry has been described in an earlier experiment report[2]. In brief the interface is illuminated from the substrate side with a monochromatic X-ray beam. After scattering from the interracial region the photons travel through the diamond crystal again on their way to the detector. This scattering geometry allows one to measure the diffraction intensities in the direction perpendicular to the surface that arise from the truncation of the crystal lattice at the interface. There are two different modes of operation. The first is to measure the specular reflectivity as a function of perpendicular momentum transfer, keeping the incident and exit angles equal. In this mode one measures the electron density profile in the direction perpendicular to the surface. Specular reflectivity y curves are very sensitive to the interracial roughness. Another mode of operation is to keep the incident angle below the critical angle for total reflection, which drastically reduces the penetration depth in the Ga liquid. This enables one to measure the intensity profiles along the crystal truncation rods (CTR's) which have a non-zero in-plane momentum transfer. The CTR's also are dependent on the interface roughness and on the atomic structure at the liquid side of the interface provided the structure exhibits long range order.

The interface was prepared, in contrast to our earlier feasibility study[2], in a dedicated ultra-high

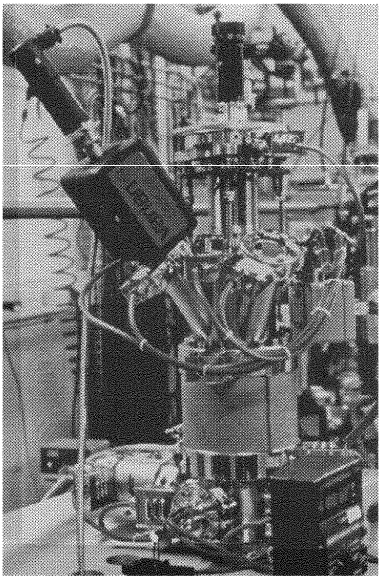

Figure 1. A photograph of the UHV set-up at the TROIKA beamline

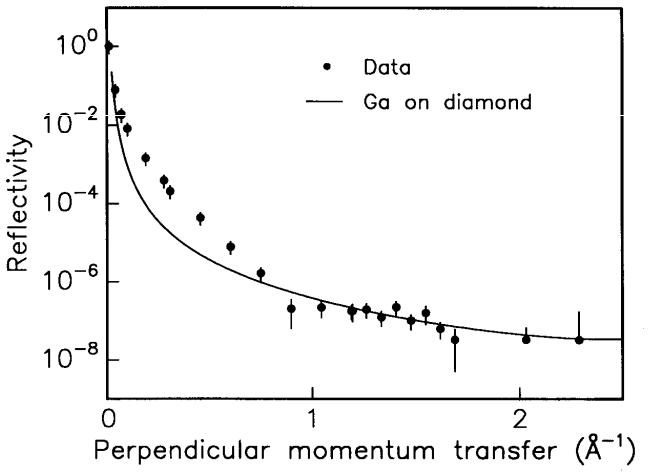

Figure 2. Reflectivity of a Ga-covered diamond surface. The model calculation (solid curve) is discussed in the text.

vacuum (UHV) set-up by depositing a drop of gallium onto the diamond surface. The UHV scattering chamber is shown in Fig. 1. It consist of one main chamber, having a base pressure of 3 x 10^{-10} mbar, fitted with a 360° Be window. The chamber was designed and manufactured at the FOM-Institute in Amsterdam. A polished diamond specimen[3] was mounted in the scattering chamber that was pumped down and fixed onto a double tilt stage on the horizontal diffractometer of the TROIKA beamline. A clean (2 **x 1)** reconstructed diamond(111) surface was prepared by flash-heating above 950° C[3]. Subsequently, a drop of liquid Ga of nominal purity 5N was decanted from the centre of the melt and was deposited onto the clean surface[4]. A photon energy of 17.058 keV (0.727 Å wavelength) was selected, which made possible measurements along the rods for vertical momentum transfers in the range o < Q_z <3 Å^{-1}.

The measured specular reflectivity is shown in Fig. 2. The intensities were measured up to a perpendicular momentum transfer of 2.5 Å^{-1}. Since further analysis is currently in progress, we have only plotted one simplified model calculation for comparison. The measured intensity distribution is compared with a reconstructed diamond(111) surface[3], covered with Ga (solid curve). The (2 x 1) reconstruction into n-bonded chains survives underneath the gallium droplet, as is suggested by the CTR profiles (with non-zero in-plane momentum transfer). In the model calculation the liquid was assumed to have a uniform density, without any ordering. Clearly, this model is too simple to offer an explanation for our observations. More realistic structural models that include planes of ordered Ga atoms at the interface are being tested.

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