ESRF	**Experiment title:** Structure of the Liquid-Metal / Oxide Surface	**Experiment number**: SI-1252
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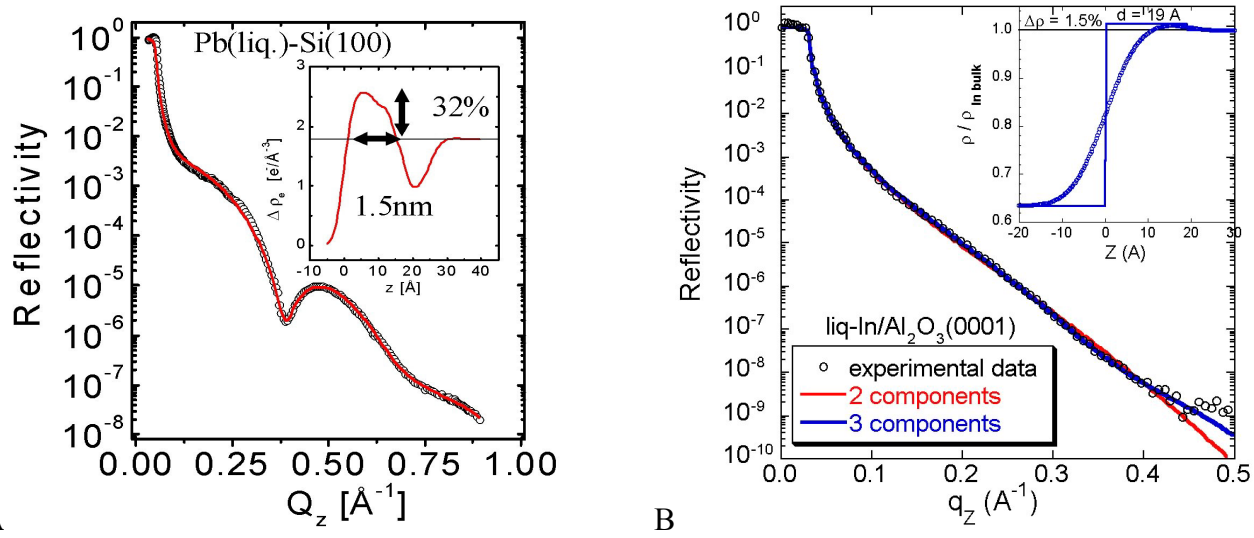
Using high-energy x-rays, the interface of In(liq.)/α-Al_2O_3(00.1) was investigated using x-ray reflectivity (XRR) and grazing angle diffraction (GAD). The structure normal to the surface can be described with a simple two-component model of a liquid-metal in contact with a hard wall substrate. In-plane measurements do not reveal a surface reconstruction but may possibly show ordering of the In atoms in the surface plane. These results contrast with the anomalies observed in prior mesaurements on liquid metals in contact with Si surfaces and support a charge transfer hypothesis across the interface of Schottky barriers.

The sample was prepared in a mobile UHV chamber at the MPI in Stuttgart prior to the allocated beamtime. The indium was cleaned by sputtering the oxide layer, and the sapphire was cleaned by flashing it to 1200 K [1]. For this project we utilized the new High-Energy MicroDiffraction endstation, commissioned within the last year at ID15A [2], which reduced the set-up time and increased the stability of the instrumentation. A 72.5 keV beam was focused (at the sample) to 6 μm (vertically) using Al compound refractive lens. Measurements at the In(liq.)/α-Al_2O_3(00.1) interface were performed at $T = T_m(In) + 20$ K.

In earlier experiments, we have conducted a systematic study of the metal/semiconductor interface on the Pb(liq.)/Si(001), Pb(liq.)/Si(111), and In(liq.)/Si(001) material systems [3,4]. From XRR measurements of these surfaces, large density oscillations normal to the surface were found in the liquid metal on a new length scale that is measured in tens of Angstroms (see Figure 1A). Currently, we attribute these generic anomalies to charge transfer effects at the interface from the metal into the semiconductor material.

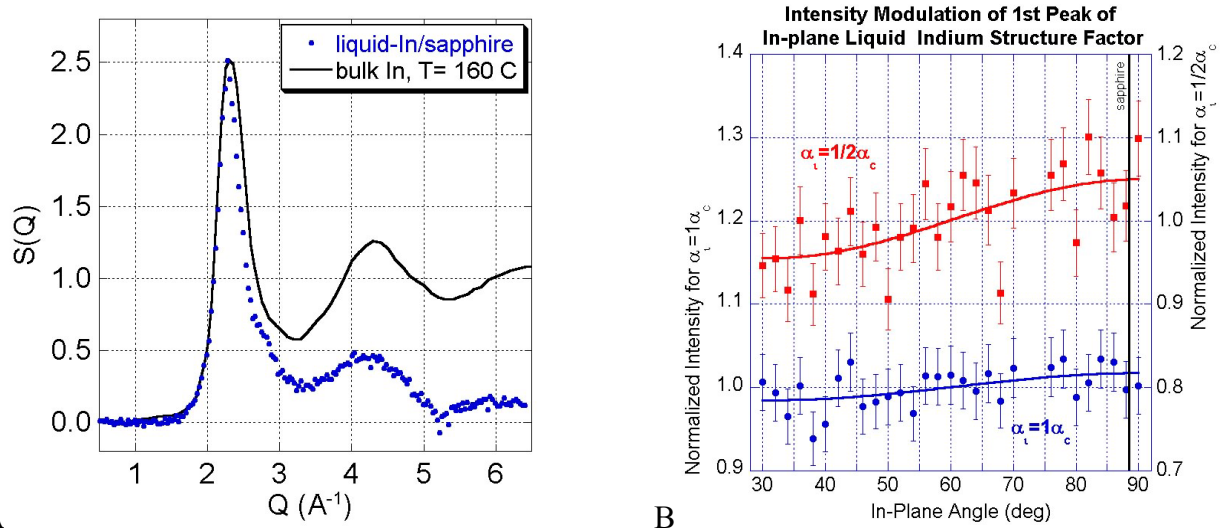
In this project we tested the charge transfer hypothesis at the interface by using an insulator material for the substrate to impose a hard wall on the liquid metal. In the XRR measurements on the In(liq.)/α-Al_2O_3(00.1) system, we did not find large density oscillations, as in the case of the semiconducting Si substrates (see Figure 1B). Modeling of the XRR data shows that the interface can be simply described with two components, sapphire and liquid-In with an interfacial roughness of 6 Å. A slight improvement in the agreement of the model with the data can be achieved by including an additional layer in the model. This results in a ~20 Å thick layer with a slight increase (1.5 %) in density compared to bulk In. This increased density can be explained by considering that the hard wall of the substrate imposes a boundary condition onto the liquid. XRR experiments accessing the vapor-liquid interface produce models of atomic layering at the free surface that extends about five layers into the liquid [5]. Due to the restricted range of q of our data, we we were not able to confirm atomic scale layering at the metal-insulator interface In(liq.)/α-Al_2O_3(00.1) .



A B

Figure 1: Reflectivity curves and models for A) liquid-Pb/Si(001), and B) liquid-In/α-Al_2O_3(0001).

The structure factor of the liquid indium near the interface was probed by GAD. A comparison with the structure factor of bulk liquid indium [6] is shown in Fig.2A. In order to search for substrate-induced ordering on the liquid side of the interface, we monitored the intensity of the 1st peak of the In structure factor (Q = 2.28 $Å^{-1}$) with respect to the substrate orientation. Different scattering depths were probed by setting the incident angle (α_i) to the interface to $0.5\alpha_c$ and to $1\alpha_c$. The preliminary analysis of the data collected over a range of 60° reveals a 5% modulation with 3-fold symmetry for $\alpha_i = ½\ \alpha_c$ (see Figure 2B). For the bulk-like structure factor at $\alpha_i = 1\alpha_c$, no discernable trend is present. The data set needs further evaluation to confirm this trend.



A B

Figure 2: Measurement of the liquid-indium in-plane structure factor at the interface: A) as a function of Q and compared to bulk In [6], and B) for the first peak in Q as a function of the substrate orientation.

References

[1] G. Renaud, Surface Science Reports **32**, 1 (1998).

[2] H. Reichert, V. Honkimäki, A. Snigirev, S. Engemann, H. Dosch, Physica B **336**, 46 (2003).

[3] H. Reichert, O. Klein, H. Dosch, M. Denk, V. Honkimäki, T. Lippmann, and G. Reiter, Nature **408**, 839 (2000).

[4] H. Reichert, M. Denk, J. Okasinski, V. Honkimäki, H. Dosch, in preparation for submission to Science.

[5] H. Tostmann, E. DiMasi, P.S. Pershan, B.M. Ocko, O.G. Shpyrko, M Deutsch, Phys. Rev. B **59**, 2 783 (1999).

[6] http://www.tagen.tohoku.ac.jp/general/building/iamp/database/scm/LIQ/periodic_table.html.