Atomic Layering Structure at the Surface of Liquid Sn

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Abstract

- We report X-ray measurements of liquid Sn which confirm the existence of atomic layering at the surface.
- Deviation of the surface structure factor for liquid Sn from the standard layering model behavior (Ga, In, K, etc) can be explained by presence of high-density layer at the surface.
- The high-density layer is an intrinsic property of Sn, rather than a result of contamination or oxidation at the surface.

Introduction

- Background
  Atomic surface layering has been theoretically predicted to occur in liquid metals by S. Rice in 1974, and has been confirmed experimentally 20 years later in a number of liquid metals such as Hg, Ga, In, K and several binary liquid metal alloys. On the other hand studies by Chacon (2001) conclude that under the right conditions non-metallic liquids could also exhibit layering.

Our results:
- We have studied the atomic layering structure of the surface of liquid Sn by the methods of X-ray reflectivity and diffuse reflectivity.
- By deconvolving the capillary wave contributions from the reflectivity measurements we were able to obtain the intrinsic surface structure factor for liquid Sn.
- The surface structure factor exhibits a peak at qz ≈ 2.3 Å−1, indicating the presence of surface-induced layering in liquid Sn, similar to that found for other metallic liquids.
- The surface structure factor deviates at low qz from a standard layering model. The deviation indicates the presence of a high-density layer at the surface.

Proof:
- The high-density layer at the surface is an intrinsic property of the liquid Sn and is not due to some Gibbs monolayer (i.e. Bi, Pb, etc) at the surface!

Deviation of the surface structure factor for liquid Sn from the expected change if contaminated.

Surface induced atomic layering is confirmed for liquid Sn. The reflectivity curve shows a fundamentally different layering from the standard layering structure found for other metals (Ga, In, K, etc).

- Energy-dispersive x-ray fluorescence and resonance x-ray reflectivity data confirm the absence of any foreign chemical species or contaminants at the surface, down to sub-monolayer quantities. This suggests that the higher-density layer is an intrinsic feature of liquid Sn.
- The fitting indicates that the low-angle reflectivity feature is consistent with an uppermost atomic layer of Sn having a 10% shorter layer spacing than the bulk’s first coordination sphere radius, resulting in a higher-than-average density at the surface.

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