Experimental Studies of Liquid Metal Surfaces

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Present research group

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Why study the surface of liquid metals?

- A large number of elements are metallic in their liquid state.
- Surfaces are always interesting.
- Interesting physics
- Applications, e.g. soldering
• An Effective potential step between liquid and vapor because ions in liquid and atoms in vapor.
• This creates a “local hard wall” simulations using this predicts layering.

X-ray Scattering From a Liquid Surface

\[ q_x = \frac{2\pi}{\lambda} \cos \beta \sin \theta \]
\[ q_y = \frac{2\pi}{\lambda} (\cos \beta \cos \theta - \cos \alpha) \]
\[ q_z = \frac{2\pi}{\lambda} (\sin \alpha + \sin \beta) \]

\[ q_{xy} = \sqrt{q_x^2 + q_y^2} \]

Total reflection if \( \alpha < \alpha_c \)

Specular reflectivity \( \alpha = \beta, \theta = 0 \)
Diffuse scattering e.g. \( \alpha \) constant, \( \theta = 0 \)
GID \( \beta = \alpha \) constant, \( \theta \) vary
Specular reflectivity

\[ \alpha = \beta, \ \theta = 0 \]

Gives information about the surface structure in z-direction

\[ \sim 10 \text{ magnitudes} \]
Diffuse scattering

$\alpha$ constant, $\theta=0$

- Temperature
- Surface tension
- Test

Used to determine surface tension
GID scan

$\beta=\alpha$ constant, $\theta$ vary

Gives information about the surface structure in xy-direction
Analysis

- The equation which describes the specular reflectivity can be broken up into three terms.

\[ R(q_z) = R_F(q_z) \times CW(q_z) \times |\Phi(q_z)|^2 \]

\[ R_F(q_z) \approx \left(\frac{q_c}{2q_z}\right)^4 \]

\[ q_c = 4\sqrt{\rho_\infty r_0 \pi} \]

\[ \Phi(q_z) = \frac{1}{\rho_\infty} \int dz \frac{d\langle \rho(z) \rangle}{dz} \exp [i q_z z] \]

The surface structure factor depends only on the electron density profile along the surface normal.
The Distorted Crystal Model (DCM)

\[ \langle \rho_{DCM}^a (z) \rangle = \frac{d}{\sigma_n \sqrt{2\pi}} \exp \left[ -\frac{(z - nd)^2}{2\sigma_n^2} \right] \]

where

\[ \sigma_n^2 = \sigma_0^2 + n \sigma_{bar}^2 \]

\[ \Phi_{DCM}^a (q_z) = \sum_{n=0}^{\infty} \exp[iq_z dn] \exp[-q_z^2 \sigma_n^2/2] \]

\[ = i q_z d \frac{\exp[-\sigma_0^2 q_z^2/2]}{1 - \exp[iq_z d] \exp[\sigma_{bar}^2 q_z^2/2]} \]

Closed form!
Modifications of the DCM

- Atomic structure factors are added.
- The parameters \((\sigma, \rho, P)\) of the outermost layer(s) does not have to follow the DCM.
- For alloys the composition in the outermost layer(s) does not have to be the same as in the bulk.

\[
\begin{align*}
\sigma_0 &= 0.4 \\
\sigma_{\text{bar}} &= 0.6 \\
d &= 2.5
\end{align*}
\]

Works well for Ga and In

\[
\begin{align*}
\sigma &= 0.6 \\
P &= -0.1
\end{align*}
\]

Needed for e.g. Sn and Bi
To calculate the electron density

\[ \frac{\langle \rho(z) \rangle}{\rho_\infty} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dq_z \left[ \frac{\Phi(q_z)}{iq_z} \exp(-iq_z z) \right] \]

How is it possible?

We know the phase
AuGe eutectic

Weight Percent Germanium

pure Au

pure Ge
From reflectivity to Structure factor

gives $\gamma$
It is possible to describe the electron density of AuGe eutectic with a slightly altered DCM.

No Gibbs absorption.
AuSi eutectic

- Abnormal (very high) intensity
  ~100 times more than expected

\[ R(q_z) = R_F(q_z) \times C'W(q_z) \times |\Phi(q_z)|^2 \]

- Bragg peaks in GID
- Crystalline lattice

The $q_{xy}^{-2}$ singularity

$$\eta = \frac{k_B T}{2\pi \gamma q_z^2}$$

Ordinary Diffuse scan

$Q_{xy}$ range $\sim 0.025 \text{ Å}$

The AuSi eutectic surface has stiffness
Earlier research

- TMDC
- Other layered materials
- SiC
- H/MgNi films

\[ E_{\text{kin}} = h\nu + E_{\text{bin}} - \phi \]
(a) Mg 2p
Mg film
- -- before
- - after
$h\nu=150$ eV
$\theta = 0^\circ$

Intensity (arb. units)

(b) Mg 2p
Mg-Ni film
- - before
- -- after
$h\nu=150$ eV
$\theta = 0^\circ$

Intensity (arb. units)
Thank You