Determination of the Cu(100)-p(3√2×√2)R45° - Sn structure using medium energy ion scattering

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Introduction

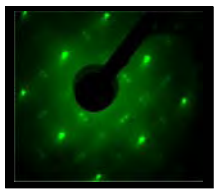
- Modified bimetallic surfaces have potential applications in heterogeneous catalysis and magnetic data storage.
- Cu adopts an f.c.c. structure at room temperature, whilst Sn adopts a tetragonal structure.
- A large atomic radii mismatch of approximately 26% exists between Cu and Sn.
- Sn deposition on Cu(100) has led to the discovery of five distinct phases at sub-monolayer Sn coverage, all of which have a complex atomic structure.

Medium energy ion scattering (MEIS)

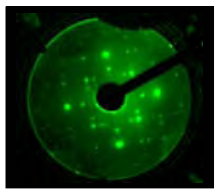
- Enables the investigation of the surface structure and properties of crystalline materials using an ion beam probe.
- Ion source generates a positively charged beam of light mass ions, typically hydrogen or helium, which can be accelerated in the energy range 50-400 keV.
- Although a very powerful technique, the high equipment cost means that there are less than ten machines world-wide.
- The Daresbury MEIS facility consists of four interconnected UHV chambers: a loading chamber; a storage chamber; the preparation chamber (including LEED, AES, sample annealing, evaporation sources, etc); and the scattering chamber in which the MEIS data is collected.
- More information at http://www.dl.ac.uk/MEIS.

Reconstructions of Sn on Cu(100)

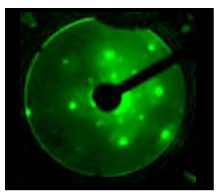
- First reported by Argile & Rhead [1], then more recently by Cafolla [2,3] and Martinez-Blanco [4]. At least 5 different reconstructions at sub-monolayer Sn coverage have been observed.



Phase I - 0.20 ML
Complex overlayer based on a p(2x2) superstructure.

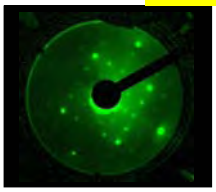


Phase II - 0.33 ML
Rotated domain p(2x6) overlayer.



Intermediate phase [4] - 0.45 ML
c(8x4) overlayer?

Phase III - 0.50 ML - p(3√2 x √2)R45° surface alloy or overlayer?

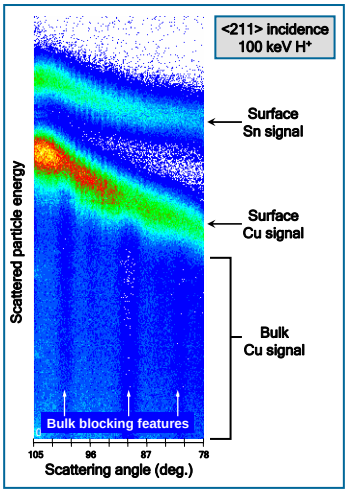


Phase IV - 0.63 ML - c(4x4)
equivalent to a tin monolayer.

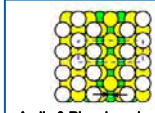
Preparation of the phase III surface

- Cu(100) surface bombarded with Ar^+ ions at 1.5 keV, followed by annealing to 550°C. (1x1) structure observed with low energy electron diffraction (LEED). Cleanliness confirmed using Auger electron spectroscopy (AES).
- Sn deposited from Knudsen cell for 35 minutes at P = 2×10^{-9} mbar. Cell temperature 1050°C. Deposition rate approximately 0.014 ML per minute.
- Phase III structure confirmed with LEED, no contamination observed in AES.

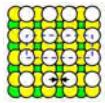
Results - Phase III



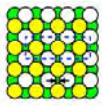
Previously proposed models of the phase III structure



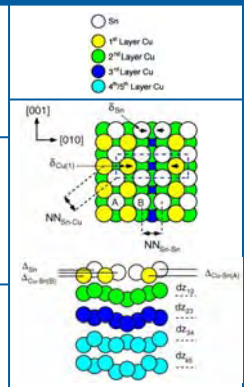
Argile & Rhead overlayer [1]



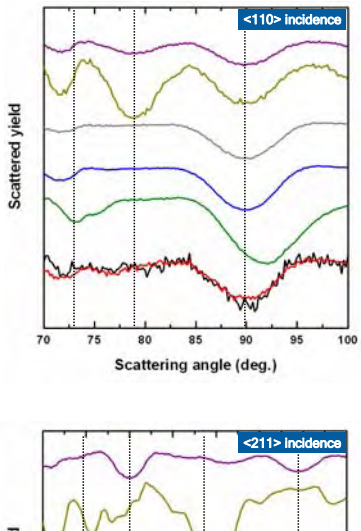
McLoughlin overlayer [3]



McLoughlin surface alloy [3]



McLoughlin surface alloy with missing Cu rows in [001] direction [3]



- Analysis of blocking curves performed using Vegas software [5].
- All models compared to experimental blocking curves in <110> and <211> incident directions. These incident geometries illuminate 1 and 2 layers of the ideal fcc(100) structure respectively.
- "Reduced" McLoughlin model corresponds to the McLoughlin surface alloy model with missing Cu rows on the surface, but with all relaxations, rumpling and lateral shifts removed.
- The initial analysis indicates that the phase III structure is closely related to the "reduced" McLoughlin model.
- Further analysis is currently being performed to optimise this structure to accurately describe the experimental data.
- The current "best-fit" is shown in red (the Warwick missing row model).
- Key features in this model include:
  - The vertical displacement of the Sn atoms relative to the Cu surface layer atoms.
  - The shift of Sn atoms towards the missing row.
  - Changes to interlayer spacings in the near-surface region.
  - Movement of Cu atoms directly below the missing row in the second and third layers

Conclusions

- 0.50 ML of Sn was deposited on a clean Cu(100) surface and led to the observation of a p(3√2 x √2)R45° LEED pattern.
- Sn signal in the MEIS data indicated no blocking and therefore no sub-surface Sn.
- Initial analysis of MEIS blocking curves discounts the previously reported model of Argile and Rhead, as well as the various solutions proposed by McLoughlin et *al.* However, the analysis does point to a surface alloy structure with missing rows running along the [001] direction.
- Optimisation of the "reduced" model structure indicates several key parameters in obtaining the final solution, including vertical and lateral displacement of Sn atoms in the surface layer, relaxations in the near-surface region and changes to the sub-surface Cu(100) structure in the vicinity of the missing row.

References

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