Determination of the sub-monolayer reconstructions of Cu(100)/Sn using medium energy ion scattering

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Introduction

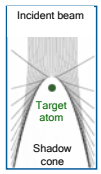
- Modified bimetallic surfaces have potential applications in heterogeneous catalysis and magnetic data storage.
- Cu adopts an f.c.c. structure at room temperature, whilst Sn adopts a tetragonal structure.
- A large atomic radii mismatch of approximately 26% exists between Cu and Sn.
- Sn deposition 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.

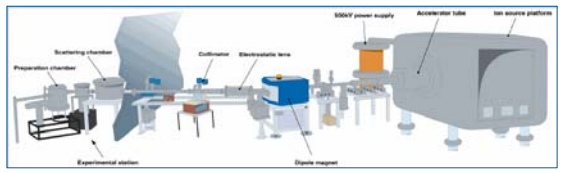
Surface preparation

- 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 at P = 2×10^{-9} mbar. Cell temperature 1050°C. Deposition rate approximately 0.014 ML per minute.
- All phases confirmed with LEED, no contamination observed in AES [1-4].

Medium energy ion scattering (MEIS)

- Enables the investigation of the surface structure and properties of crystalline materials using an ion beam probe and double-alignment of the resulting shadow cones.
- 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.
- 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.

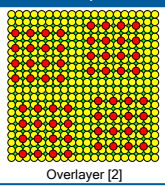


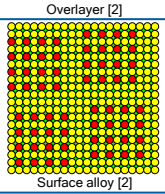


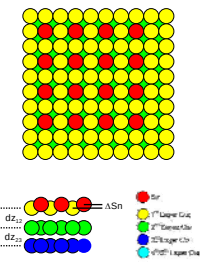
More information at http://www.dl.ac.uk/MEIS.

Phase I results

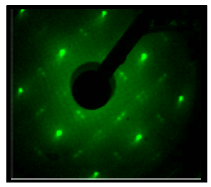
Proposed models of the phase I structure

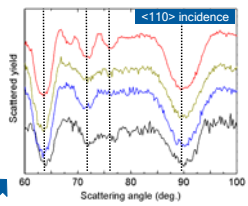

Overlayer [2]

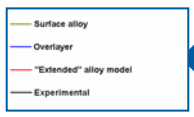

Surface alloy [2]

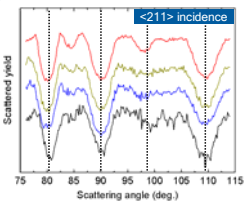


Simplified surface alloy - still with p(2x2) superstructure, but with MEIS insensitive domain structure removed


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



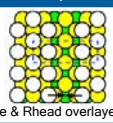




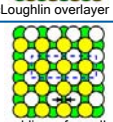
- Analysis of blocking curves performed using Vegas software [5].
- All models compared to experimental blocking curves in <110> and <211> incident directions.
- Initial analysis indicates that a surface alloy is more likely.
- "Simplified" surface alloy model corresponds to the surface alloy model but with the different domains removed. MEIS is insensitive to these different domains, so the simplified model is used for analysis because it has a smaller number of atoms.
- The "Extended" alloy model contains that same p(2x2) superstructure as the simplified model, but with 5x5 structures in place of the 4x4.
- Using the simplified alloy model as a starting point, three key parameters can be identified:
  - 1. The first interlayer spacing (dz_{12})
  - 2. The second interlayer spacing (dz_{23})
  - 3. Displacement of Sn atoms out of plane of Cu atoms (ΔSn)

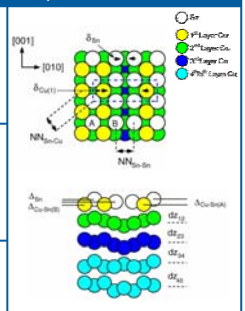
Phase III results

Proposed models of the phase III structure

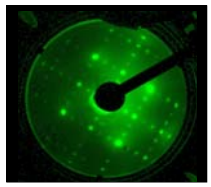

Argile & Rhead overlayer [1]

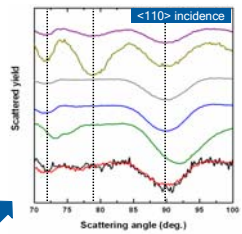

McLoughlin overlayer [3]

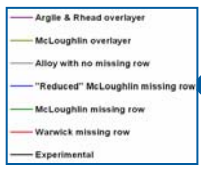

McLoughlin surface alloy [3]

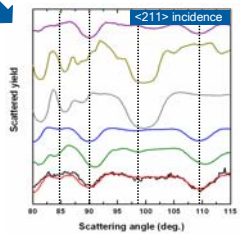


McLoughlin surface alloy with missing Cu rows in [001] direction [3]


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







- Analysis of blocking curves performed using Vegas software [5].
- All models compared to experimental blocking curves in <110> and <211> incident directions.
- "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.
- Analysis is being performed to further optimise this structure, with the current "best-fit" 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

- Sn was deposited on a clean Cu(100) surface and led to the observation of p(2 x 2) and p(3√2 x √2)R45° LEED patterns.
- Sn signal in the MEIS data indicated no blocking and therefore no sub-surface Sn.
- Phase I results indicate that a surface alloy is more likely, and that the size of the p(2x2) based structures has an effect on the blocking dips seen.
- Initial analysis of Phase III 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" Phase III 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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