High Resolution
Coaxial Impact Collision Ion Scattering Spectroscopy

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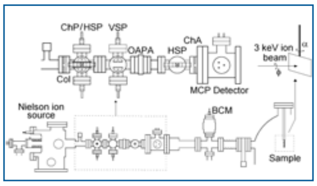
CAICISS

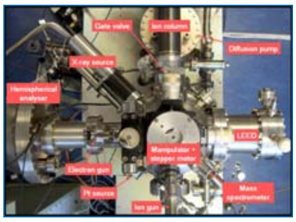
- Coaxial impact collision ion scattering spectroscopy.
- Offers the chance to probe the atomic structure and composition of surfaces with a high degree of surface specificity.
- Time-of-flight ⇨ composition information.
- Shadow cones and interaction potential ⇨atomic structure.
- Extract polar angle vs backscattered intensity profile for each element in the sample.
- Use computer simulations to derive a model for the surface using FAN code [1].

Experimental Setup

- Analysis chamber equipped with LEED, XPS, sputter gun, evaporation sources, gas cracker and bolt-on CAICISS system.
- 5-axis manipulator capable of x-y-z translation and both polar and azimuthal sample rotation.
- Two modes of sample heating: RT - 300 °C via resistive heating only; 300 °C to 800 °C via resistive heating and biasing the sample up to 350 V.
- Polar angle rotation automated in both 0.9° and 1.8° steps. Smaller than 0.5° steps are possible with manual operation. Manual azimuthal control to better than 0.1°.
- CAICISS utilises a Nielson ion source ⇨ He^+ or Ne^+, 1.0 keV ≤ E_0 ≤ 3.4 keV.
- Steering plates sweep beam across chopping aperture ⇨ time resolution: 10-200 ns (typically 60 ns is used).
- Beam spot ~ 1.0 mm diameter at sample using 3 keV He^+.
- Detect ions and neutrals scattered through 179° ± 1° with a microchannel plate detector.
- Collect backscattered intensity vs time-of-flight at a range of polar angles. Extract intensity vs polar angle plots and analyse using the FAN code [1].



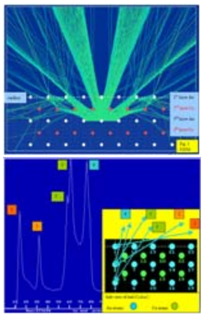
- Schematic diagram (left) and photograph (right) of the Warwick CAICISS system. From left-to-right: the ion source, ion column and analysis chamber. In the schematic diagram, the beam steering and detector section of the column is shown in the upper part of the figure, whilst the polar (α) and azimuthal (ϕ) rotation axes are shown in the upper-right.



- The main analysis chamber, showing the surface science tools used on the system and their relative locations.

FAN Simulation Code [1]

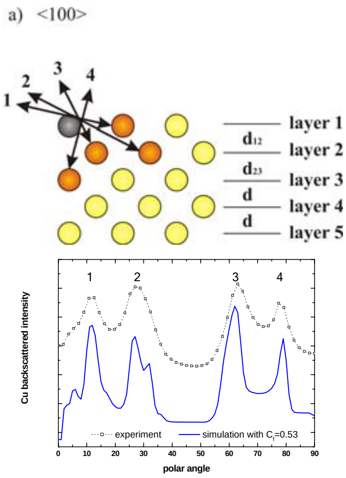
- Enables fast simulations of particle trajectories (ions & neutrals).
- Designed specifically for backscattering techniques.
- Capable of simulating both polar and azimuthal crystal rotations.
- Trial structures can incorporate three different atomic species, relaxations and other features.
- Enables choice of interaction potential (TFM or ZBL) and screening factor.
- Includes temperature and neutralisation effects, as well as off-axis scattering.
- Does not include inelastic energy losses along the trajectory.

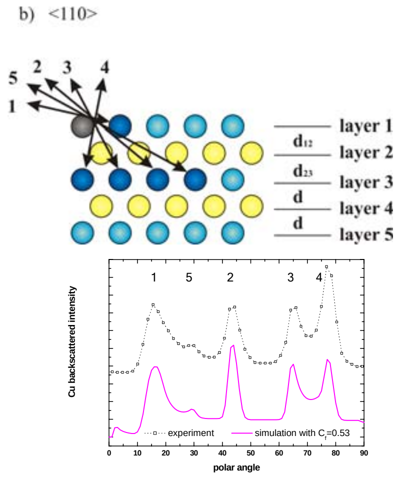


Results and Analysis

- Clean Cu(100)

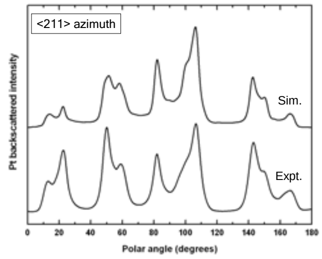
Best fit of data in both the <100> & <110> azimuths obtained for C_f = 0.53, d_{12} = 1.74 Å, d_{23} = 1.83 Å and d = 1.807 Å



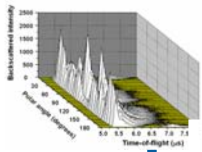


- Clean Pt(111)

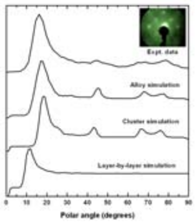
Relative to bulk Pt(111) structure, outermost interlayer spacing, Δ_{12}, found to be relaxed by +2% and second interlayer spacing, Δ_{23}, expanded by +6%.



- Pt on Cu(100), 0.55 ML coverage



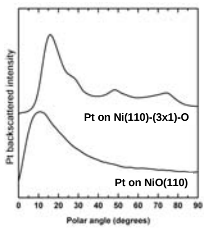
- Raw data collated in the form of a 3D plot of backscattered intensity vs polar angle and ToF.

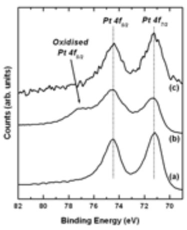


- Intensity vs polar angle plot for each element is compared to many surface models using FAN.
- FAN shows that Pt on Cu(100) at RT forms a surface alloy [3].

- Pt on NiO(110) and Ni(110)-(3x1)-O surfaces, Pt coverage ~ 0.30 ML [5]

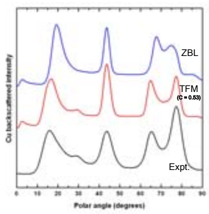
- CAICISS shows difference in the initial growth of Pt on the Ni(110)-(3x1)-O and NiO(110) surfaces.
- Peaks in excess of 25° indicate sub-surface Pt. Therefore an alloy is formed on (3x1)-O surface.
- Surface layer peak shifted to 10° for Pt on NiO(110), suggesting a Pt layer on top of the oxidised surface.
- XPS also indicates a Pt film on NiO (c), with no bonding seen between Pt and O atoms, in contrast to the oxidation of Pt(111) (b). (a) was taken from a clean Pt(111) surface.



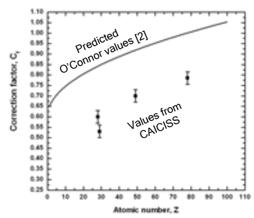


The ion-surface interaction potential [6]

- Two different models for the ion-surface interaction are commonly used in low energy ion scattering.
- Thomas-Fermi-Molière (TFM) with a tunable correction factor (C) to the screening length (from O'Connor [2]), or the "universal" Ziegler-Biersack-Littmark (ZBL).
- From work on clean Cu(100) and other surfaces, ZBL is not appropriate for CAICISS. Screening length corrections from O'Connor are too high to re-create experimental results. Work is ongoing in to this issue, with many surfaces being investigated at different incident energies.



Element	O'Connor C factor	CAICISS C factor
Cu	0.85	0.53 ± 0.03
Ni	0.84	0.60 ± 0.03
In	0.92	0.70 ± 0.03
Pt	1.00	0.78 ± 0.03



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