Re-evaluating the ion-atom interaction potential in low energy ion scattering

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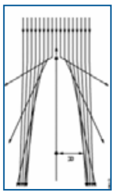
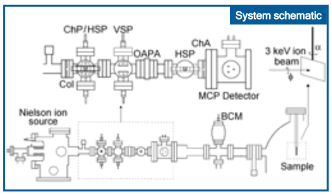
Introduction

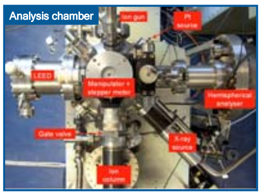
- Although elemental identification and compositional information only requires the binary collision model, the ion-surface interaction potential (IP) is a prerequisite for undertaking any detailed structural analysis with ion beam techniques, including CAICISS (coaxial impact collision ion scattering spectroscopy).
- The most frequently used IPs are the Thomas-Fermi-Molière (TFM) and the "Universal" Ziegler-Biersack-Littmark (ZBL) Potential [1].
- Especially at low energies, these potentials have to be modified to reproduce experimental results. This is typically done by multiplying the screening length by a correction factor, C_f.

Coaxial impact collision ion scattering spectroscopy (CAICISS)

- Coaxial impact collision ion scattering spectroscopy [2] offers the chance to probe the structure and composition of surfaces with a high degree of surface specificity. The technique has been used to study a range of surface science problems, including real-time growth, surface reconstructions and metal oxide / alloy formation.
- Time-of-flight ⇒ composition information from binary collision. Shadow cones ⇒ structural information from ion-target interaction. In these experiments an incident beam of He^+ with an energy of 3 keV was used.
- Intensity vs. polar angle plot for each element are compared to simulations generated using the FAN code [3].
- More information at http://uk.geocities.com/phrxaj/CAICISS.htm .







Screened Coulomb Potentials [1]

- Thomas Fermi Molière (TFM):

$$\Phi_{TFM}(x) = 0.35 \cdot \exp(-0.3x) + 0.55 \cdot \exp(-1.2x) + 0.1 \cdot \exp(-6x)$$

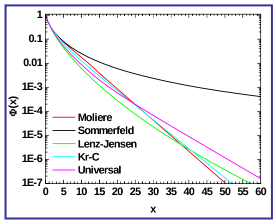
with $x = r/a$, *where* $a = C_f \cdot a_{Screening}$

C_f ... constant factor, of the order of 0.65 - 1.25 [2]

or $C_f = 0.045 \cdot (\sqrt{Z_1} + \sqrt{Z_2}) + 0.54$ [3]

and $a_{Screening}$ being either $a_{Firsov} = \frac{0.88534 \cdot a_0}{(\sqrt{Z_1} + \sqrt{Z_2})^{2/3}}$

.... or $a_{Lindhard} = \frac{0.88534 \cdot a_0}{(\sqrt{z_1^{2/3} + z_2^{2/3}})}$.

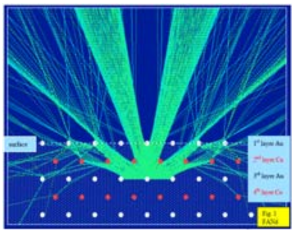


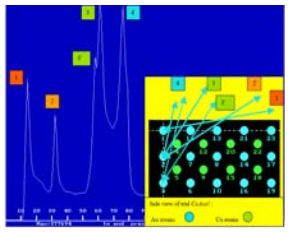
Other Potentials:

- ZBL / "Universal"
- Lenz - Jensen
- Sommerfeld
- Kr - C

FAN Simulation Code [3]

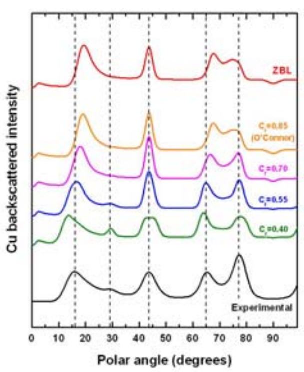
- Enables fast simulations of trajectories (ions & neutrals). Designed specifically for backscattering techniques.
- Simulations in both polar & azimuthal rotations. Trial structures can incorporate three different atomic species.
- Enables choice of interaction potential (TFM or ZBL) and screening factor. Includes temperature and neutralisation effects, as well as off-axis scattering.

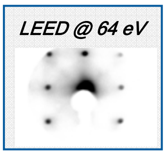




CAICISS results

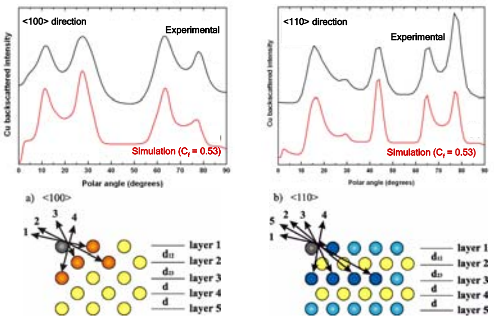
The clean Cu(100) surface [4]



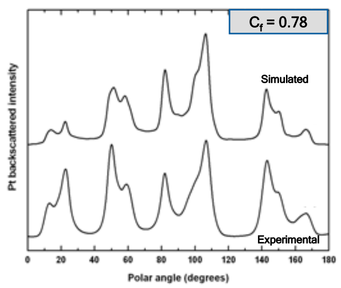


Note: The vertical scales on all plots have been normalised for easier visualisation.

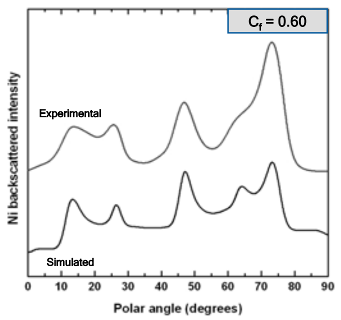
Best replication of the experimental data from the Cu(100) surface in both the <100> and <110> directions given by C_f = 0.53.



Clean Pt(111) [5]

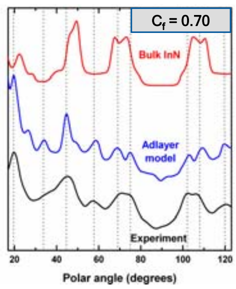


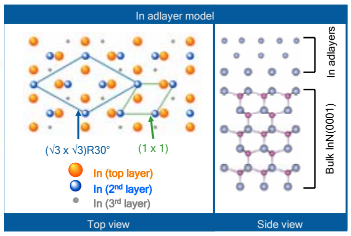
Ni(110)-(3x1)-O [2]



InN(0001) [6]

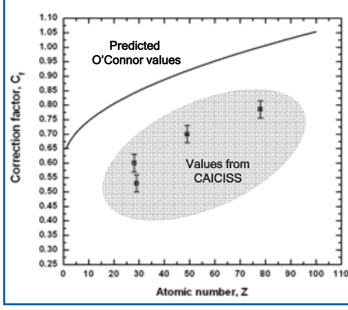
- Recent high-resolution XPS data taken at NCESS facility suggests In-polarity InN has a contracted layer termination, in analogy to GaN(0001). This is supported by CAICISS analysis using a correction factor of 0.70.





- For more information, see our poster dedicated to this investigation.

Summary [7]



Element	Ni	Cu	In	Pt
O'Connor C_f prediction [3]	0.84	0.85	0.92	1.00
C_f CAICISS value	0.60	0.53	0.70	0.78
Difference	0.24	0.32	0.22	0.22

- All values derived from experiments performed using 3 keV He^+.
- At this point in time, the root cause of this discrepancy remains unknown. Experiments investigating the effects of incident ion mass and energy are to be conducted in the near future.

References

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