How accurately are the interaction potentials known in ion scattering spectroscopy?

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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.
- Especially at low energies, these potentials have to be varied to reproduce experimental results. This is typically done by multiplying the screening length by a correction factor, *C*.

CAICISS

- Coaxial impact collision ion scattering spectroscopy [1] offers the chance to probe the structure and composition of surfaces with a high degree of surface specificity.
- Technique has been used to study a range of surface science problems, including real-time growth, surface reconstructions and surface alloy formation.
- Time-of-flight ⇒ composition information from binary collision.
- Shadow cones ⇒ structural information from ion-target interaction.
- Extract intensity vs. polar angle plot for each element.
- Use computer simulations to derive a model for the surface.

Screened Coulomb Potentials

Thomas Fermi Molière (TFM):

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

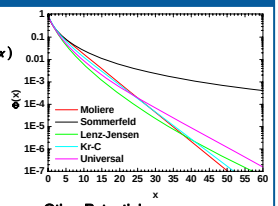
with $x = r/a$, where $a = C_f \cdot a_{Screening}$

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

or $C_f = 0.042 \cdot \left(\sqrt{Z_1} + \sqrt{Z_2}\right) + 0.57$ [3]

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

.... or $a_{Lindhard} = \frac{0.88534 \cdot a_0}{\left(\sqrt[3]{Z_1} + \sqrt[3]{Z_2}\right)^{1/2}}$.

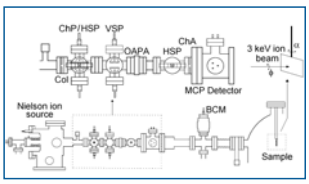


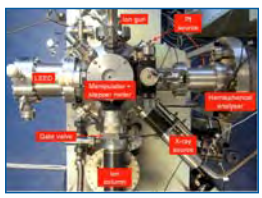
Other Potentials:

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

Experimental Details

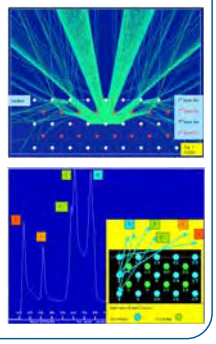
- CAICISS, LEED and XPS for chemical and structural information.
- Sputter ion gun, thermal gas cracker and target heating up to 800°C.
- All samples prepared using cycles of Ar^+ bombardment and annealing.
- Use FAN code (see below) to interpret CAICISS data [4].





FAN Simulation Code [4]

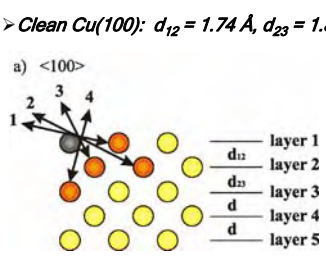
- Enables fast simulations of particle trajectories (ions & neutrals).
- Designed specifically for backscattering techniques.
- Capable of simulating polar and azimuthal crystal rotations.
- Trial structures can incorporate three different atomic species.
- Enables choice of interaction potential (TFM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

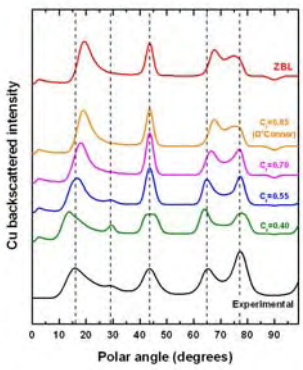


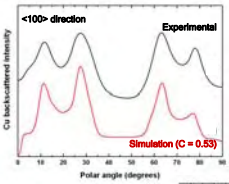
Results

- *Clean Cu(100): d_{12} = 1.74 Å, d_{23} = 1.83 Å, d = 1.807 Å*

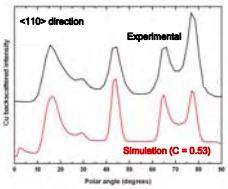
LEED @ 64 eV



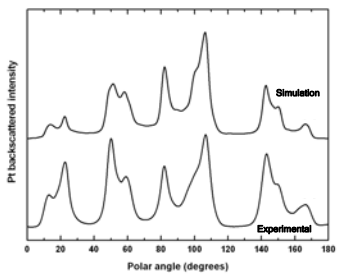




Best replication of the experimental data from the Cu(100) surface in both the <100> and <110> directions given by C_f = 0.53.

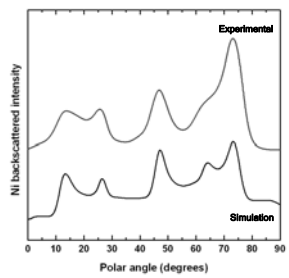


- *Clean Pt(111) [5]*



- Best fit produced using C_f = 0.78

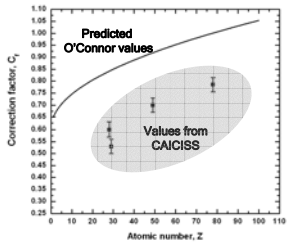
- *Ni(110)-(3x1)-O [6]*



- Best fit produced using C_f = 0.60

Element	O'Connor C factor [3]	CAICISS C factor
Ni	0.84	0.60 ± 0.03
Cu	0.85	0.53 ± 0.03
In	0.92	0.70 ± 0.03
Pt	1.00	0.78 ± 0.03

- All values derived from experiments using 3 keV He^+.



Conclusions

- "Universal" ZBL potential and O'Connor correction to the screening length in the TFM potential are both inadequate in describing CAICISS data recorded using 3 keV He^+ ions.
- Correction factor for Firsov screening length was determined to be lower than predicted by O'Connor for the Cu(100), Pt(111), InN(0001) and Ni(110)-(3x1)-O surfaces.
- ZBL potential underestimates the electron screening at large distances and this leads to incorrect peak positions in the CAICISS polar angle scans.
- To fully understand these results, further work is required at different primary energies (1-5 keV) on more surfaces in order to establish the target mass and primary energy dependencies of the correction factor.

References

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