HOW ACCURATE ARE INTERACTION POTENTIALS AT LOW ENERGIES?

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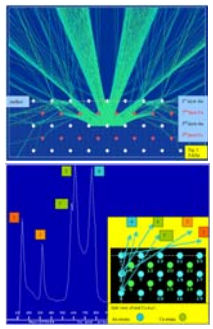
INTRODUCTION

- The Interaction Potential (IP) is a prerequisite for undertaking any detailed structural analysis with Ion Beam Techniques.
- The most frequently used IPs are the Thomas-Fermi-Moliere (TFM) and the Ziegler-Biersack-Littmark (ZBL) or "Universal" Potential.
- Especially at low energies these potentials have to be adjusted to reproduce experimental results. This is typically done by adjusting the screening length by a small multiplicative factor.
- CAICISS (coaxial impact collision ion scattering spectroscopy) is a technique capable of analysing surface structure and composition BUT structural information requires knowledge of IP.

The simulation package FAN

- Enables fast simulations of particle trajectories to be calculated(ions & neutrals).
- Designed specifically for backscattering techniques (unlike Monte Carlo simulations).
- Capable of simulating both 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.



Screened Coulomb Potentials:

TFM:

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

with $x = r/a$.

$a = C_f \cdot a_{Screening}$, with C_f …constant factor of the order of 0.65 - 1.25 [1]

or $C_f = 0.042\cdot(\sqrt{Z_1}+\sqrt{Z_2}) + 0.57$ [2]

and $a_{Screening}$ being either a_{Firsov} or $a_{Lindhard}$

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

ZBL:

$$\Phi_{ZBL}(x) = 0.1818\cdot\exp(-3.2x) + 0.5099\cdot\exp(-0.9423x) + 0.2802\cdot\exp(-0.4029x) - 0.02817\cdot\exp(-0.2016x)$$

with $x = r/a_{ZBL}$ and $a_{ZBL} = \frac{0.88534\cdot a_0}{Z_1^{0.23}+Z_2^{0.23}}$.

$a_0 = 0.529$Å.

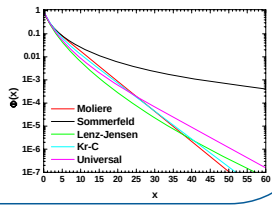
Other Potentials:

$$\Phi_{Sommerfeld}(x) = \left(1+\left(\frac{x}{12^{2/3}}\right)^{0.8034}\right)^{-\frac{3}{0.8034}}$$

$$\Phi_{Lenz-Jensen}(x) = \exp^{(-c)}\cdot\left[1 + c + 0.3344\cdot c^2 + 0.0485\cdot c^3 + 2.647\cdot 10^{-3}\cdot c^4\right]$$

with $c = 3.11126\cdot\sqrt{x}$

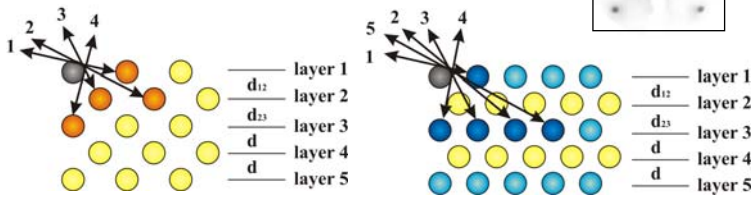
$$\Phi_{Kr-C}(x) = 0.190945\cdot\exp(-0.278544\cdot x) + 0.473674\cdot\exp(-0.637174\cdot x) + 0.335381\cdot\exp(-1.919249\cdot x)$$

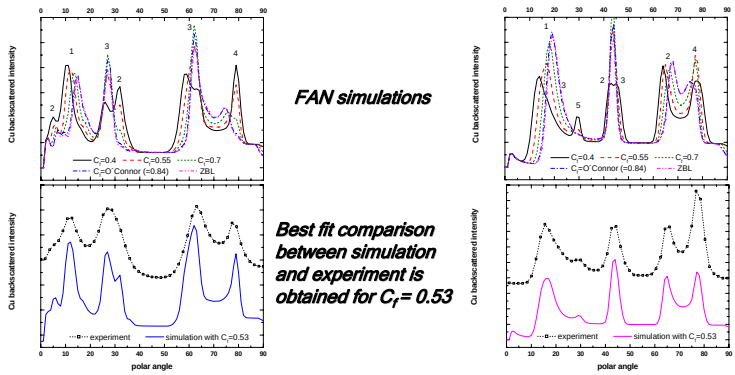


RESULTS

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

LEED @ 64 eV



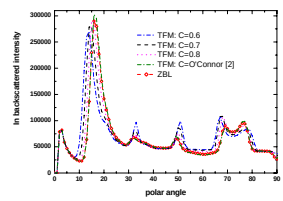


FAN simulations

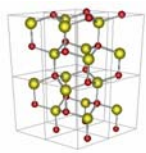
Best fit comparison between simulation and experiment is obtained for C_f = 0.53

Compound semiconductors:

Indium nitride (InN)



Wurtzite: a = 3.54 Å
c = 5.70 Å

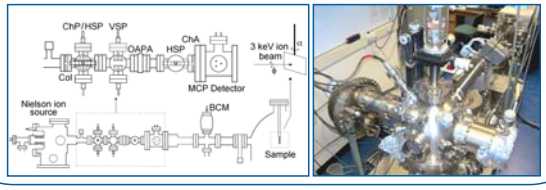


Coaxial Impact Collision Ion Scattering Spectroscopy (CAICISS)

- Offers the chance to probe the structure and composition of surfaces with a high degree of surface specificity.
- Time-of-flight ⇒ composition information.
- Shadow cones ⇒ structural information.
- Extract intensity vs. polar angle plot for each element.
- Use computer simulations to derive a model for the surface.

EXPERIMENT

- CAICISS, LEED and XPS
- Sputter ion gun, thermal gas cracker and target heating up to 800°C
- Use FAN code to interpret CAICISS data [3]



CONCLUSIONS

- Cu(100) was used as a trial structure: contraction of 3.9% between layer 1 and layer 2 and expansion of 1.3% between layer 2 and layer 3.
- Correction factor for Firsov screening length was determined to be C_f = 0.53 to adequately describe our experimental results.
- ZBL potential under estimates the electron screening at large distances and this leads to incorrect peak positions in the CAICISS polar angle scans.

REFERENCES

[1] T. Fauster, Vacuum 38 (1988) 129 and references therein.
[2] D.J. O'Connor and J.P. Biersack, Nucl. Instr. and Meth. B 15 (1986) 14.
[3] H. Niehus, W. Heiland and E. Taglauer, Surf. Sci. Rep. 17 (1993) 213.

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