Quantification of second layer contributions in LEIS

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ATOM- UND OBERFLÄCHEN PHYSIK

Motivation:

- Low Energy Ion Scattering (**LEIS**) widely used tool to analyse surface composition and structure.
- Noble gas ions as projectiles → supreme surface sensitivity due to efficient neutralization inside the target.
- Depending on target / projectile / energy: contribution from deeper layers possible.
- **Is it possible to quantify contributions from second layer?**
- **How does the relative contribution from different layers depend on the primary energy?**

Ion yield Y^+:

$$Y^+ = I_0 \cdot n \cdot \underbrace{\frac{d\sigma}{d\Omega} \cdot d\Omega \cdot \eta}_{Y_B} \cdot P^+$$

I_0 : Number of projectiles

n : Surface areal density

$\frac{d\sigma}{d\Omega}$: Scattering cross sec.

P^+ : Ion fraction

$d\Omega$: Detector solid angle

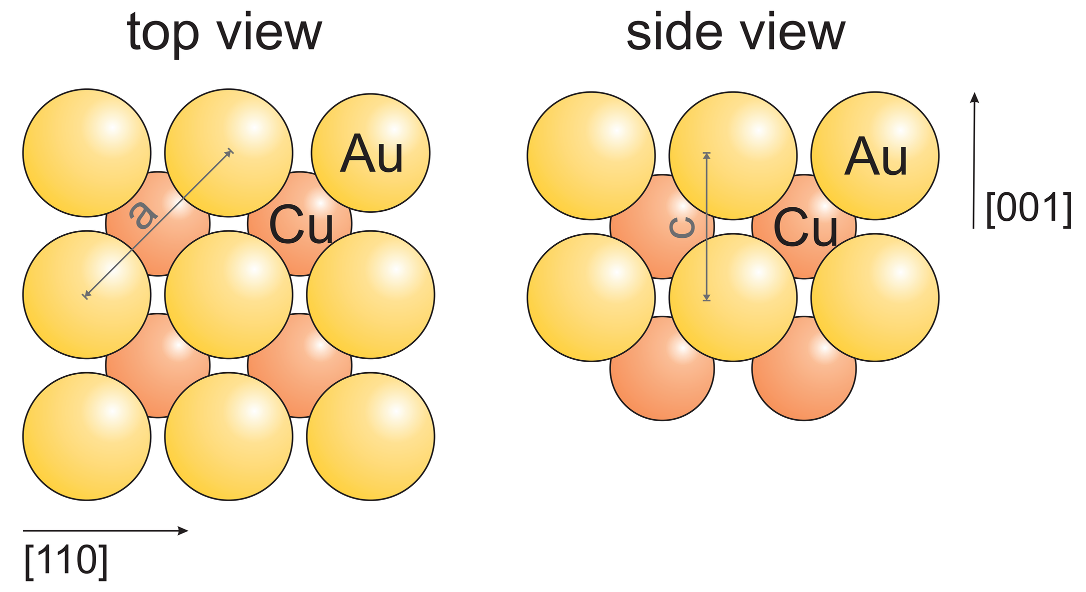
η : Detector efficiency

Y_B : Backscattered yield

For a given target, one can obtain the ratio of ion fractions from the ratio of ion yields when the ratio of backscattered yields is known

$$\frac{Y^+_{Cu}}{Y^+_{Au}} = \frac{Y_{B,Cu}}{Y_{B,Au}} \cdot \frac{P^+_{Cu}}{P^+_{Au}}$$

Target: $Cu_{0.5}Au_{0.5}(001)$



$Cu_{0.5}Au_{0.5}(001)$: tetragonal geometry

a = 3.875, c/a = 0.924

alternating layers of Au and Cu

Perfect sample to investigate 2[nd] layer contributions. Large mass difference between Cu and Au permits to decompose ion signal.

2 keV He^+ scattered from CuAu(001)

Experiment

TOF-LEIS set-up: ACOLISSA

postaccelaration to separate ions

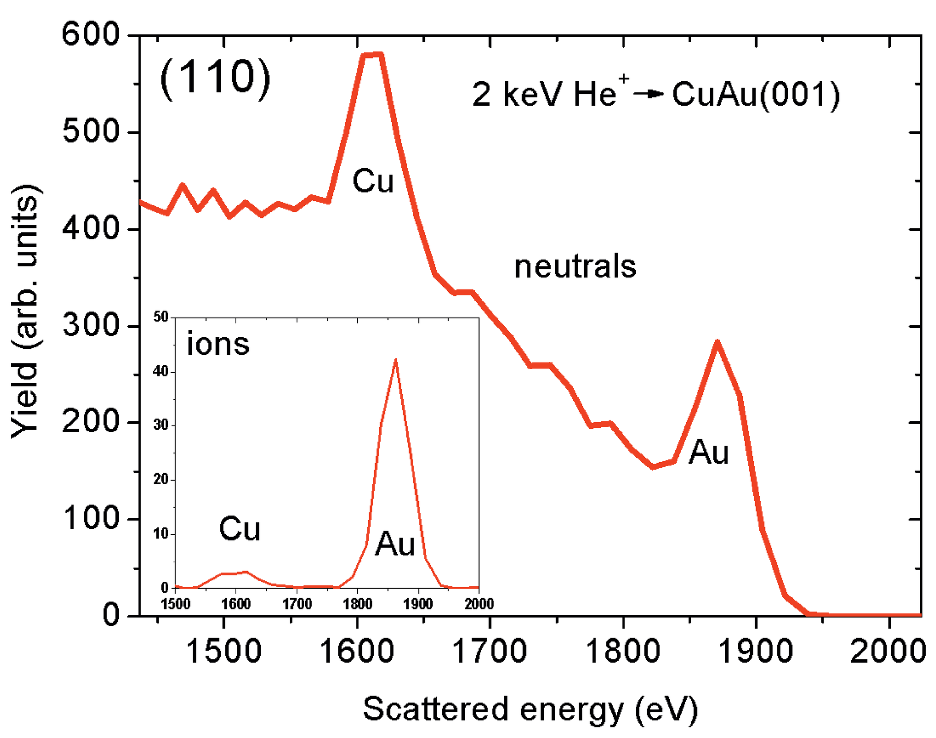


Fig. 1: Experimental spectrum of 2 keV He ions scattered from CuAu(001) - [110] azimuth. Au and Cu can be separated easily.

Evaluation

$$\frac{Y^+_{Cu}}{Y^+_{Au}} \qquad \frac{Y_{B,Cu}}{Y_{B,Au}}$$

$$\frac{P^+_{Cu}}{P^+_{Au}} \simeq 0.21$$

P^+_{Au} can be determined from experimental spectrum. This permits to explicitly calculate P^+_{Cu}:

$$P^+_{Au} = 0.196 \qquad P^+_{Cu} = 0.042$$

From comparison of scattering cross sections for Cu and Au with the simulated spectrum a significant focussing effect can be deduced:

$$\frac{d\sigma_{Au}}{d\Omega} \Big/ \frac{d\sigma_{Cu}}{d\Omega} = 3.1 \qquad \frac{Y_{B,Au}}{Y_{B,Cu}} = 2.1$$

MD-Simulation

Simulation package: KALYPSO

interaction: ZBL Potential

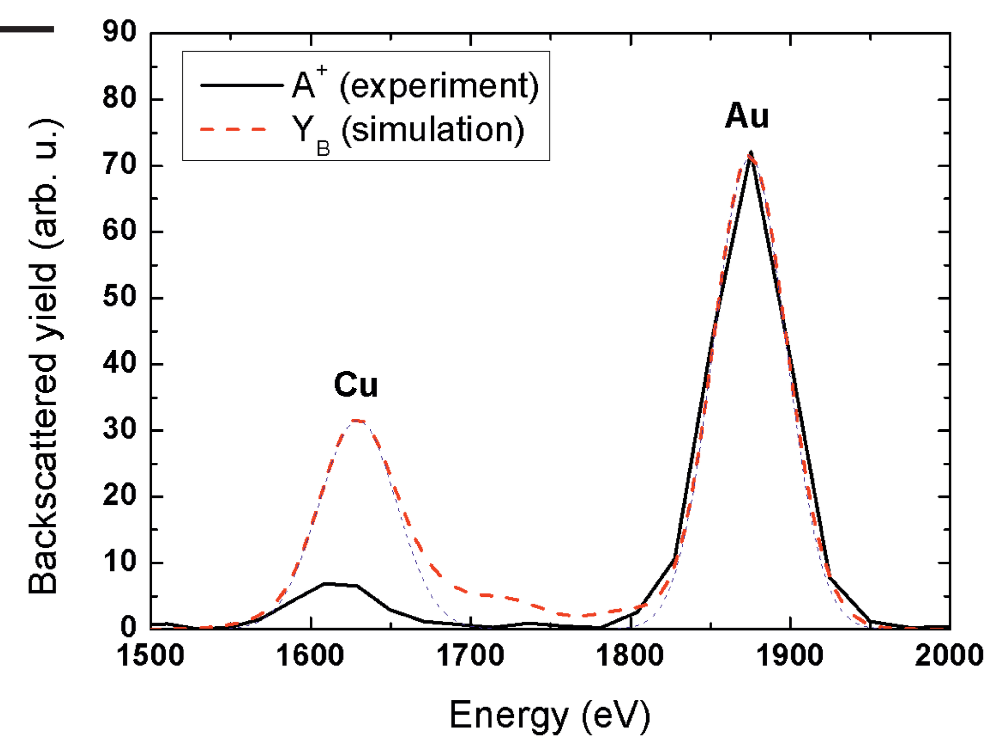


Fig. 2: Simulated spectrum of backscattered particles without consideration of charge exchange

Energy dependence:

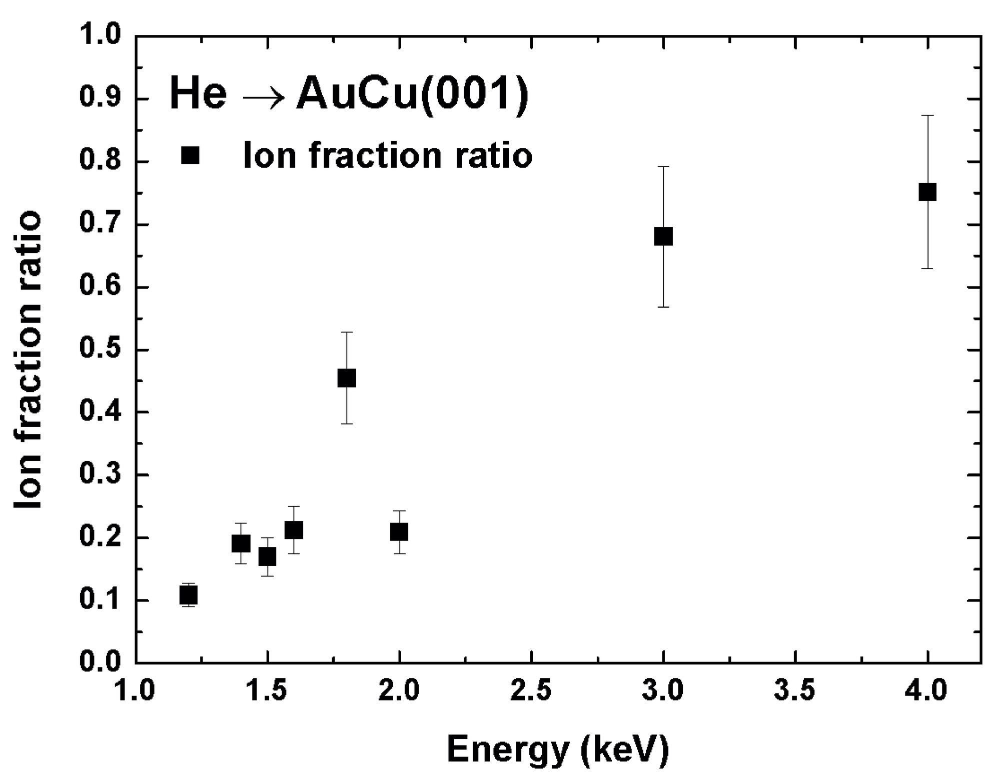


Fig. 3: Ion fraction ratio evaluated for different energies. Note, how the ratio and consequently the relative contributions from the 2[nd] layer increase with energy.

Charge exchange:

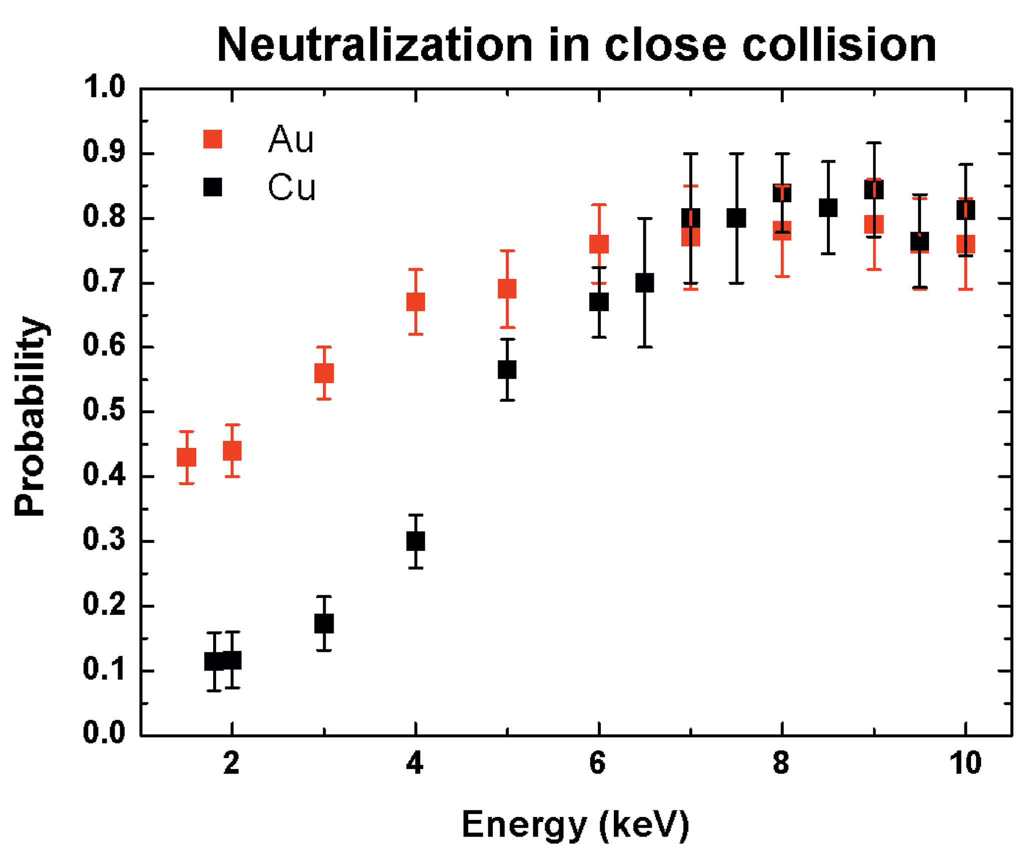


Fig. 4: Probability of neutralization in a close collision for He/Au and He/Cu. One can see the substantial difference, especially at energies < 5 keV.

Conclusion:

- **For low energies, information is reduced to outermost atomic layers, with only small relative contributions from 2[nd] layer atoms.**
- **At higher energies, ion signal can contain substantial contribution from 2[nd] layer.**
- **Increased contributions from 2[nd] layer due to different neutralization probabilities in close collisions.**
- **Determination of information depth in LEIS experiments requires accurate knowledge of charge exchange processes.**

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