8. Ion scattering techniques

8.1 Low Energy Ion Scattering (LEIS or ISS)

Setup: - Incident monoenergetic ion beam (0.5 – 3 keV, He⁺ / Ne⁺ / Ar⁺) scatters at surface  
- Energy-resolved measurement of scattered ions at fixed exit angle

Theory: - If $E > 0.5$ keV, interaction time of scattering event short (< 1 ps)  
interation energy large compared to local binding energy  
very little electron transfer (negligible neutralization)  
→ ion scattering event simply determined as two-body inelastic collision  
of ion with mass $M_1$ and energy $E_0$ with surface atom of mass $M_2$  
- Simple rules of momentum and energy conservation (classical mechanics!) determine

\[
\frac{E_1}{E_0} = (1+A)^{-2} \left[ \cos \theta_1 \pm (A^2 - \sin^2 \theta_1)^{1/2} \right]^2 \\
\frac{E_2}{E_0} = 4A(1+A)^{-2} \cos^2 \theta_2 \quad \text{and} \quad A = \frac{M_2}{M_1} > 1
\]

- Since energy is conserved, unique relation between scattered particle energy $E_i$ at fixed angle $\theta_i$ and ratio of masses $A$
- Mass resolution determined by energy width of peaks in spectrum
  - energy resolution and collimation of incident beam
  - acceptance angle of detector (larger collection angle yields lower resolution, but higher signal/noise)
  - detection angle (large $\theta_1$ yields highest resolution)
  - mass ratio (small $A$ yields highest resolution, but $A > 1$ even for lighter surface species)

$\rightarrow$ He$^+$ / Ne$^+$ / Ar$^+$ and $\theta_1 = 90^\circ$ often chosen

- Highly surface specific, because of
  - elastic shadow cone (largest for lower energy ions)
  - ion neutralization (also suppresses multiple scattering)

- Quantification difficult, because
  - differential cross-section depends on (unknown) ion-atom interaction potential
  - neutralization

$\rightarrow$ ICISS / RBS ?!
8.2 Secondary Ion Mass Spectrometry (SIMS)

Setup:
- Bombard surface with high energy (10-100 keV), massive ions (Ar⁺)
- Detect particles sputtered away from surface with mass spectrometer
- Measure positive and/or negative ions (<1%):
  - positive/negative SIMS
- Ionize neutrals (>99%) by postirradiation: SNMS
- Sputtered particles arise predominantly from topmost surface layers as end result of collisional cascade with low kinetic energies (~10 eV)

Modes of operation:

static SIMS (low sputter rates, <10 Å hr⁻¹, “non-destructive”)
- semi-quantitative chemical composition (mass spectrum of ions), not affected by differential sputtering!
- some structural information (cracking patterns from fragments)
- spatial information on chemical composition from ion microprobe or ion microscopy mode (~100 nm resolution)

dynamic SIMS (high sputter rates, up to 100 µm hr⁻¹)
- surface cleaning
- depth profiling in conjunction with other surface sensitive technique (affected by preferential sputtering!)
8.3 Pros and cons of ion scattering techniques

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- Very surface sensitive (static SIMS can trace impurities at <1% ML concentration)
- Straightforward experiment (fingerprinting)
- Spatially resolved information in microprobe/microscope modes
- Used in both depth-profiling (dynamic SIMS) or „non-destructive“ mode (static SIMS, LEIS)
- Works for insulators and conductors

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- Intrinsically destructive (even in static-SIMS/LEIS ions can cause chemistry and/or interlayer mixing)
- Rich SIMS spectra difficult to rationalize
- Absolute quantification of spectra extremely difficult
  LEIS: unknown ion-atom interaction potential, neutralization
  SIMS: uncertainties in ionization probabilities, sputtering yields, mass spectrometer sensitivity
- Requires vacuum