FONDAZIONE BRUNO KESSLER

ECT*
EUROPEAN CENTRE FOR THEORETICAL STUDIES IN NUCLEAR PHYSICS AND RELATED AREAS

UNIVERSITY OF TRENTO - Italy
Department of Civil, Environmental and Mechanical Engineering

Monte Carlo simulation of Secondary Electron Yield for Noble metals

Martina Azzolini, Nicola M. Pugno, Simone Taioli, Maurizio Dapor

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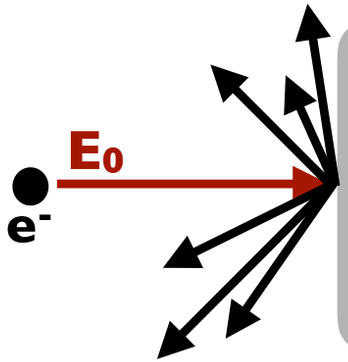
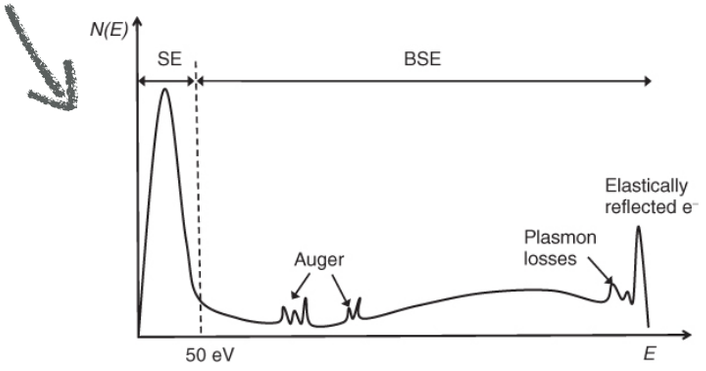
OUTLINE

- Description of the Monte Carlo computational model to simulate electron transport:
  - Initial energy distribution
  - Elastic scattering
  - Inelastic scattering, ionization and secondary electrons generation
  - Emission condition
  - Path length and choice of the interaction kind
- Comparison between calculated and experimental emission spectra of Cu and secondary electron yield of Cu, Ag and Au.
- Conclusion and further perspectives

Monte Carlo simulation of electron transport in solid targets

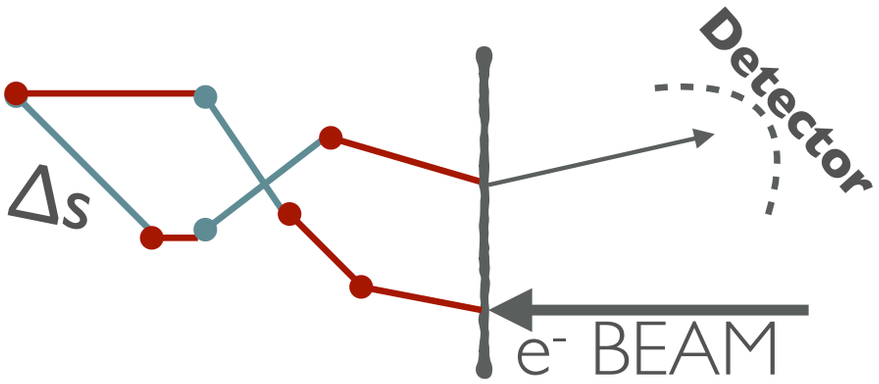


Trajectories calculation



Monte Carlo simulation:

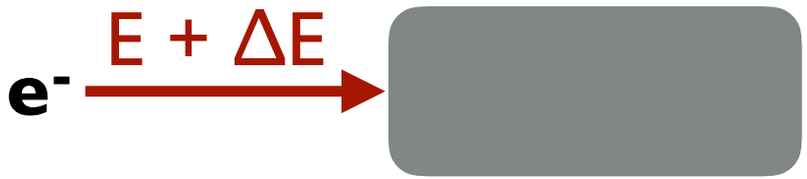
- Generation of random numbers
- Calculation of scattering probabilities of interactions
- Repetition of the calculation



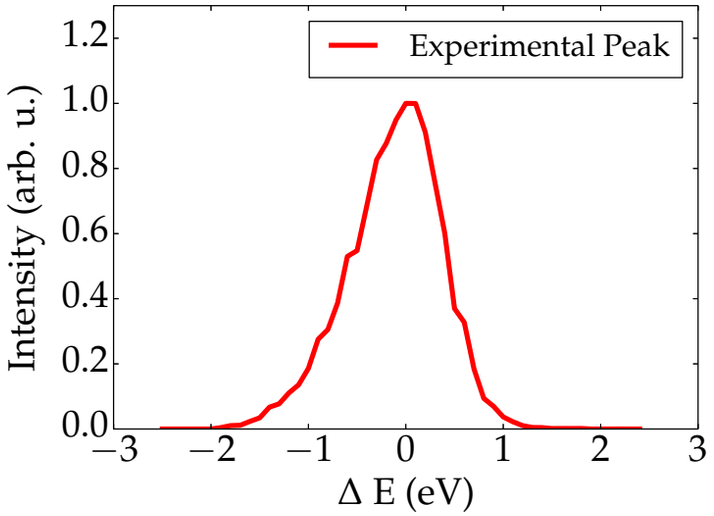
- Step between interactions
- Elastic scattering: direction change
- Inelastic scattering: energy loss, direction change, ionizations and secondary electron generation
- End of the electron trajectories: kinetic energy lower than threshold, emission of electron (overcome the energy barrier represented by the work function)

D. C. Bell, N. Erdman, Low Voltage Electron Microscopy: Principles and Applications, Wiley, 2013

Beam kinetic energy



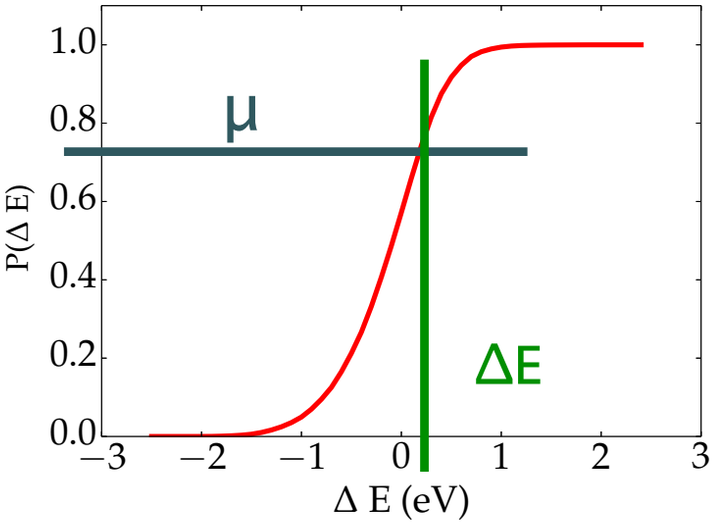
Experimental elastic peak *
(taken on a graphite reference sample)



$$Area = \int_{E_-}^{E_+} f(\Delta E)d(\Delta E)$$

ΔE = ?

$$P(\overline{\Delta E}) = \frac{1}{Area}\int_{E_-}^{\overline{\Delta E}} f(\Delta E)d(\Delta E)$$



Generation of a random number μ, uniformly distributed in the interval [0,1]

$$\mu = P(\overline{\Delta E})$$

The corresponding value of ΔE is the energy correction to apply

* Experimental data by M. Angelucci, R. Larciprete, R. Cimino

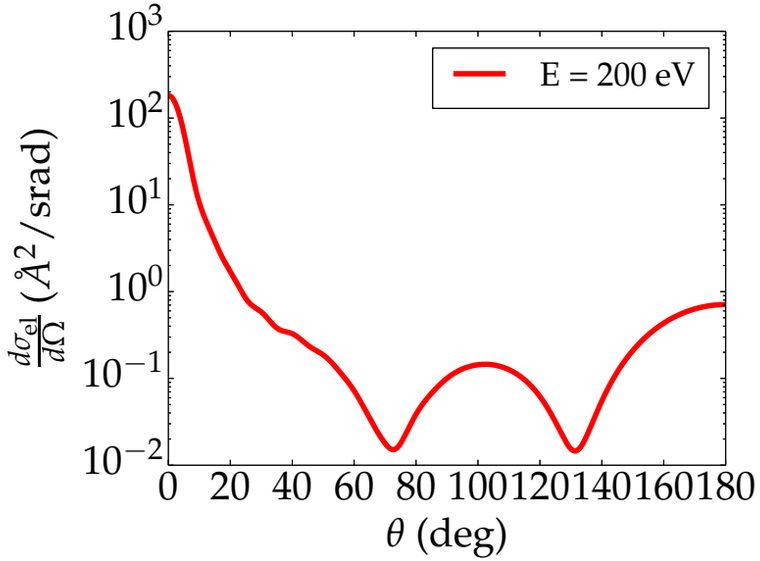
Elastic scattering:

- Angular deviation

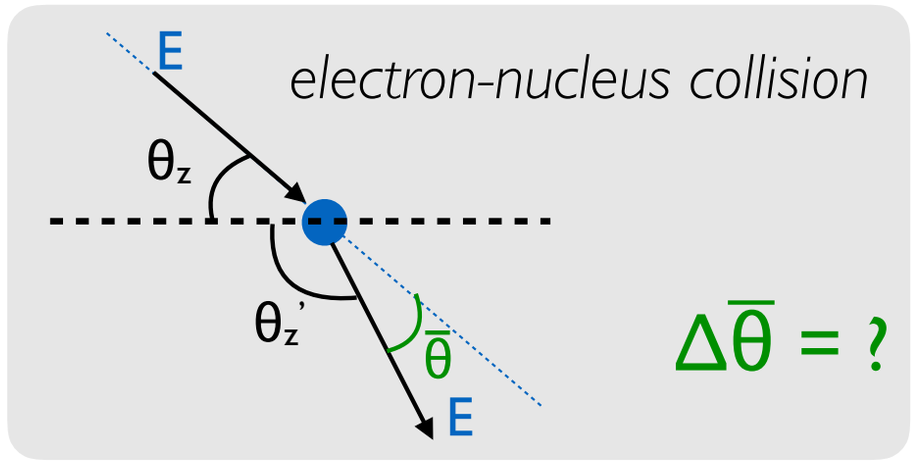
Mott theory with the potential by Salvat.

Differential elastic scattering cross section of copper:

$$\frac{d\sigma_{\mathrm{el}}}{d\Omega} = |f|^2 + |g|^2$$

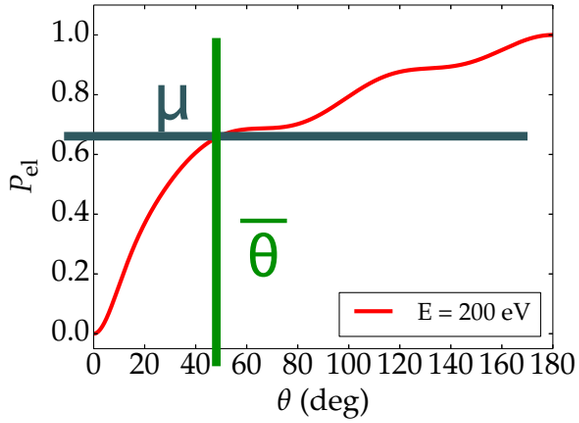


$$\sigma_{el} = 2\pi \int_0^{\pi} \frac{d\sigma_{el}}{d\theta} sin(\theta) d\theta$$



Cumulative elastic probability

$$P_{\mathrm{el}}(\bar{\theta}, E) = \frac{2\pi}{\sigma_{\mathrm{el}}(E)} \int_0^{\bar{\theta}} \frac{d\sigma_{\mathrm{el}}(E)}{d\theta} \sin\theta d\theta$$



Generation of a random number μ, uniformly distributed in the interval [0,1]

The corresponding value of θ is the trajectory deviation angle

N. Mott, The scattering of fast electrons by atomic nuclei, Proc. R. Soc. London, Ser. A 124 (794) (1929) 425.

F. Salvat, J. Martinez, R. Mayol, J. Parellada, Analytical Dirac-Hartree-Fock-Slater screening function for atoms (Z=1-92), Phys. Rev. A 36 (1987) 467–474

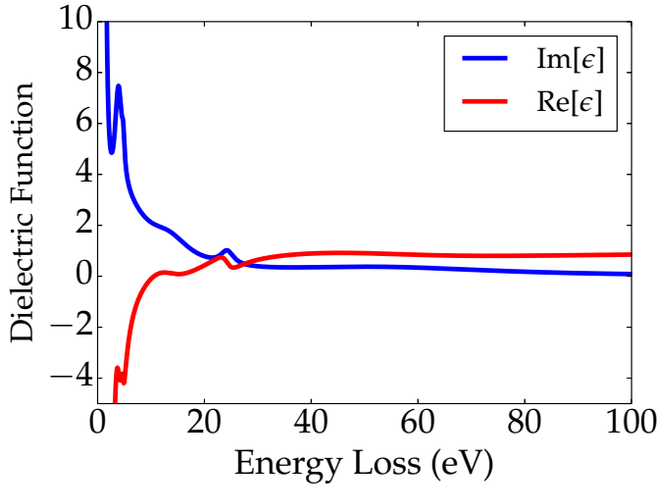
Inelastic scattering

- Angular deviation
- Energy loss
- Ionization + secondary electron generation

Ritchie dielectric theory and dielectric function obtained by experimental Reflection electron energy loss spectra by Werner et al. It reports the contribution of surface plasmon excitation.

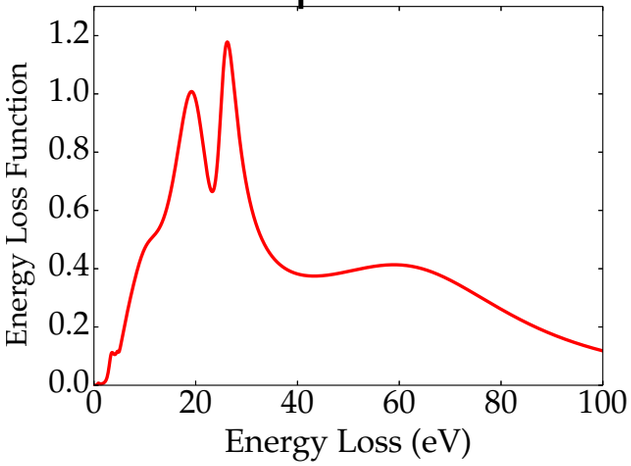
$$\epsilon(q, W)$$

Dielectric function of copper in the optical limit



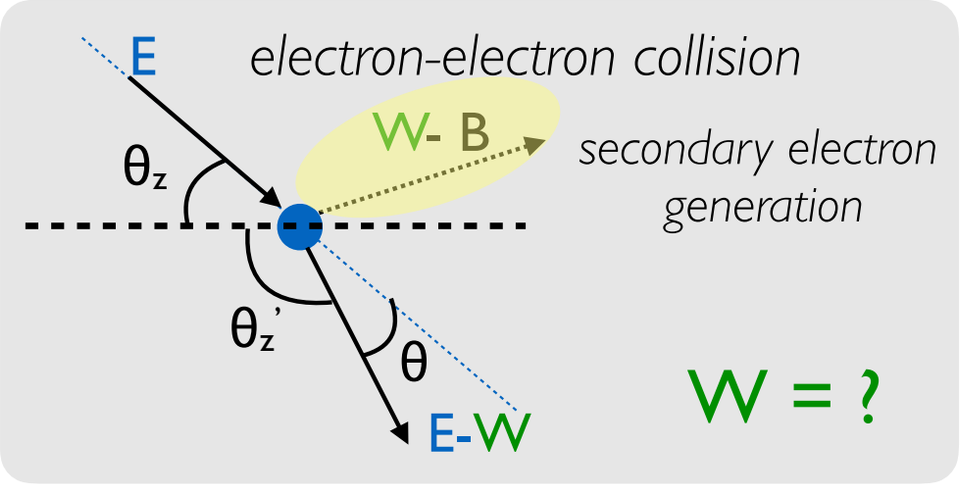
$$\mathrm{Im}\left[-\frac{1}{\epsilon(q, W)}\right]$$

Energy loss function (ELF) of copper in the optical limit



R. H. Ritchie, Plasma losses by fast electrons in thin films, Phys. Rev. 106 (1957) 874.
W. S. Werner, K. Glantschnig, C. Ambrosch-Draxl, Optical constants and inelastic electron-scattering data for 17 elemental metals, Journal of Physical and Chemical Reference Data 38 (4)(2009) 1013–1092.

Inelastic scattering



Differential inelastic scattering cross section

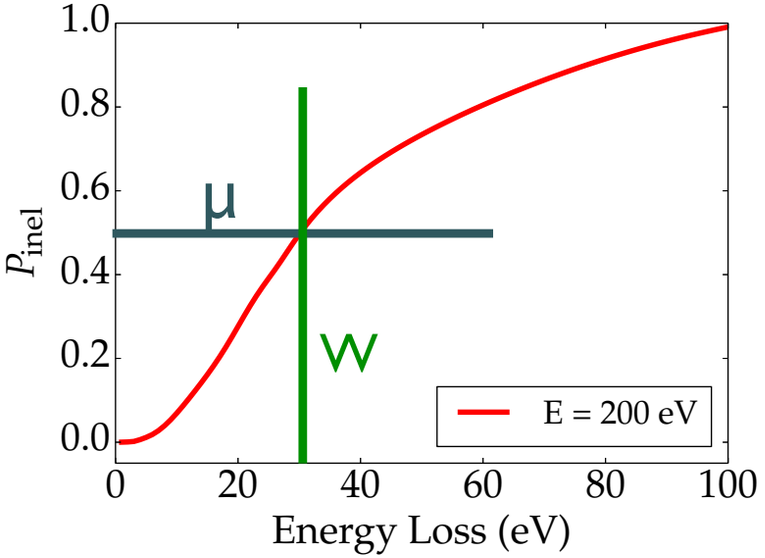
$$\frac{d\sigma_{inel}}{dW} = \frac{1}{N\pi a_0 E}\int_{q-}^{q+} Im\left[-\frac{1}{\epsilon(q,W)}\right]\frac{dq}{q}$$

Cumulative inelastic scattering probability:

$$P_{inel}(W,E) = \frac{1}{\sigma_{inel}}\int_0^W \frac{d\sigma_{inel}}{dW'}dW'$$

Generation of a random number μ, uniformly distributed in the interval [0,1].

The corresponding value of W is the energy loss.

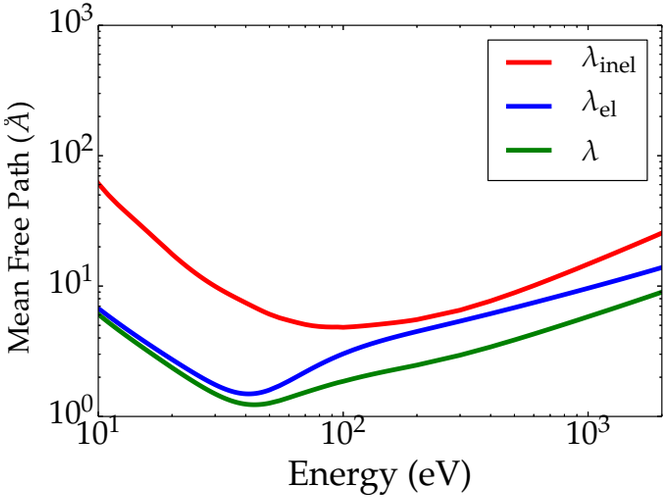


If the energy loss is higher than the first ionization energy (B) of the target atom, a secondary electron is generated.
Also its trajectory is calculated.

Step length

λ is the overall mean free path (Cu)

$$\lambda^{-1} = \lambda_{inel}^{-1} + \lambda_{el}^{-1} = N(\sigma_{inel} + \sigma_{el})$$



Δs is the step length between two subsequent collisions

$$\Delta s = -\lambda \ln(\mu)$$

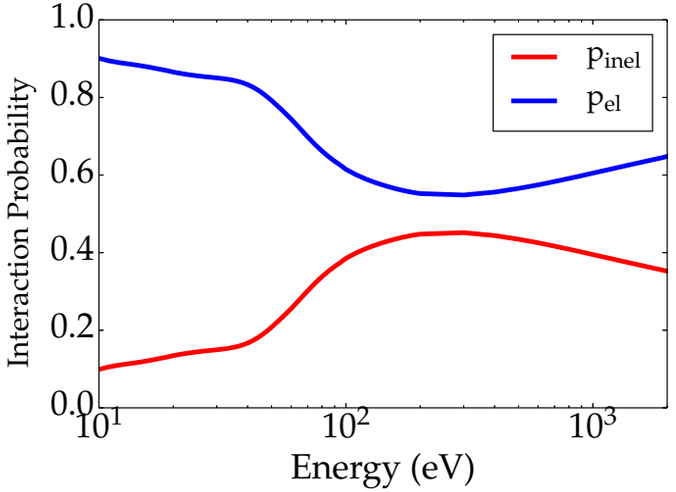
where μ is a random number uniformly distributed in the interval [0,1]

Kind of interaction

Another random number μ (uniformly distributed in the interval [0,1]) is generated. Its value is compared to p_{el}, where:

$$p_{\mathrm{el}} = \frac{\lambda}{\lambda_{\mathrm{el}}}$$

If μ < p_{el} the interaction will be elastic, otherwise inelastic.



Electron emission from the surface

The electron has to overcome the energy barrier represented by the work function.

The emission condition to be satisfied is:

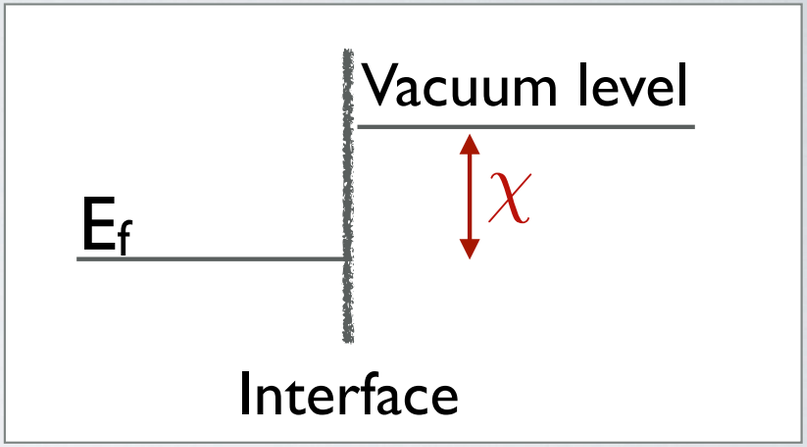
$$E\cos^2\theta \geq \chi$$

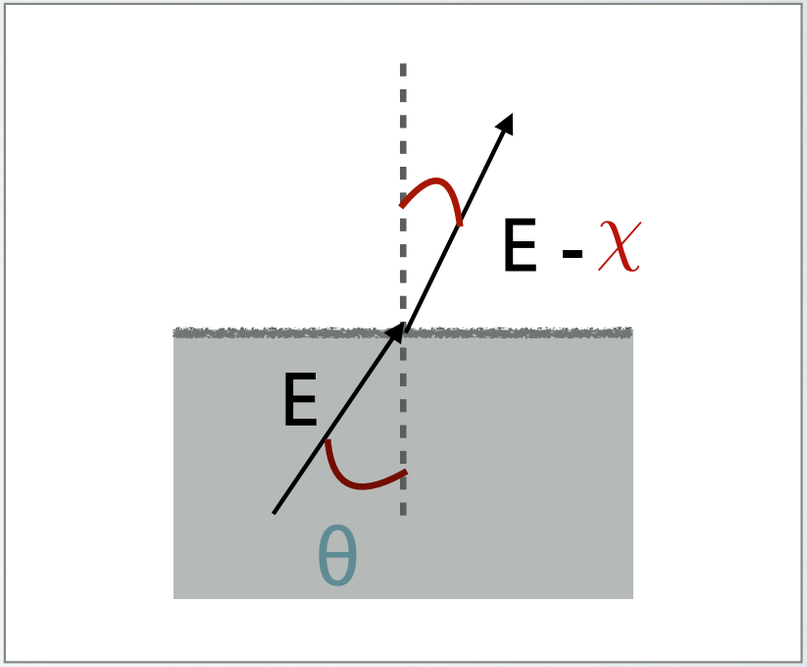
The transmission coefficient is calculated as:

$$T = \frac{4\sqrt{1-\chi/(E\cos^2\theta)}}{\left[1+\sqrt{1-\chi/(E\cos^2\theta)}\right]^2}$$

In order to decide if the electron will be emitted, another random number μ (uniformly distributed in the interval [0,1]) is generated.

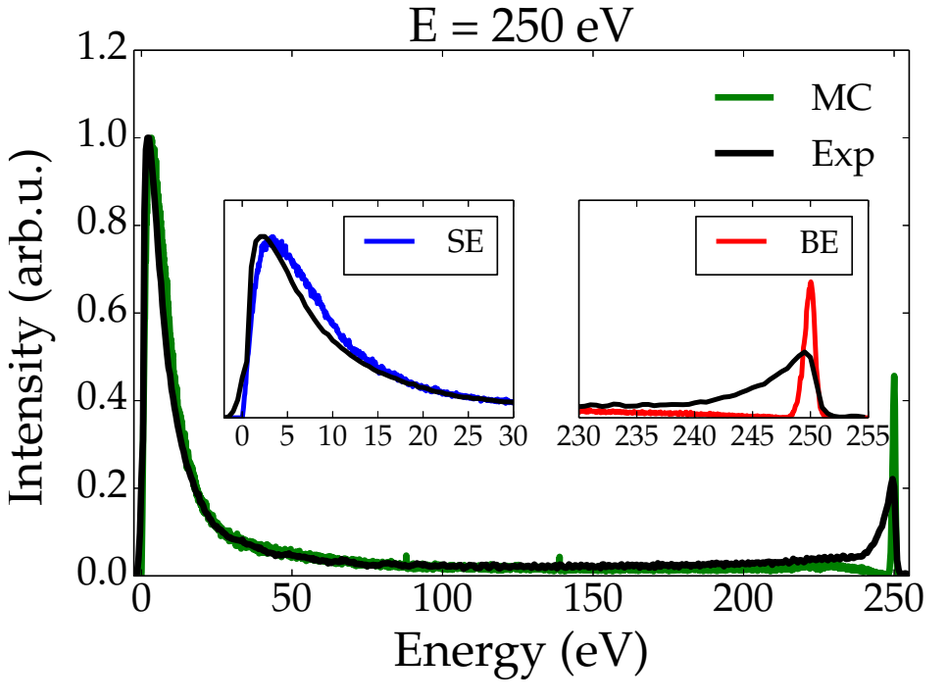
If μ < T the electron will be emitted and collected and its energy value is stored.

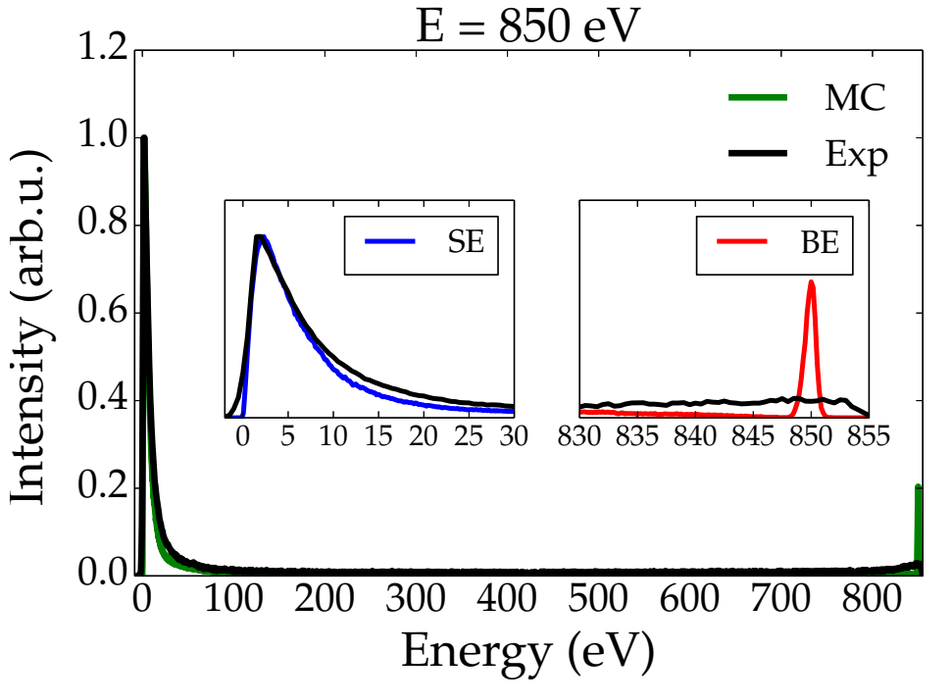




Emission spectra of Cu

10^7 trajectories





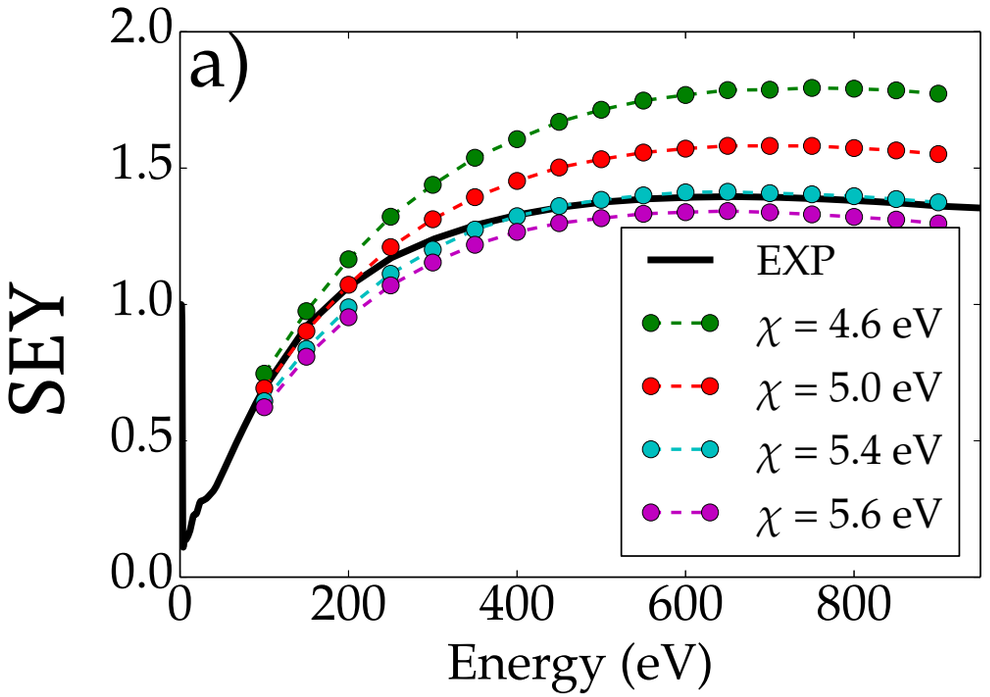
Spectra normalized at a common height of the SE peak.
Preliminary experimental data by M. Angelucci, R. Larciprete, R. Cimino

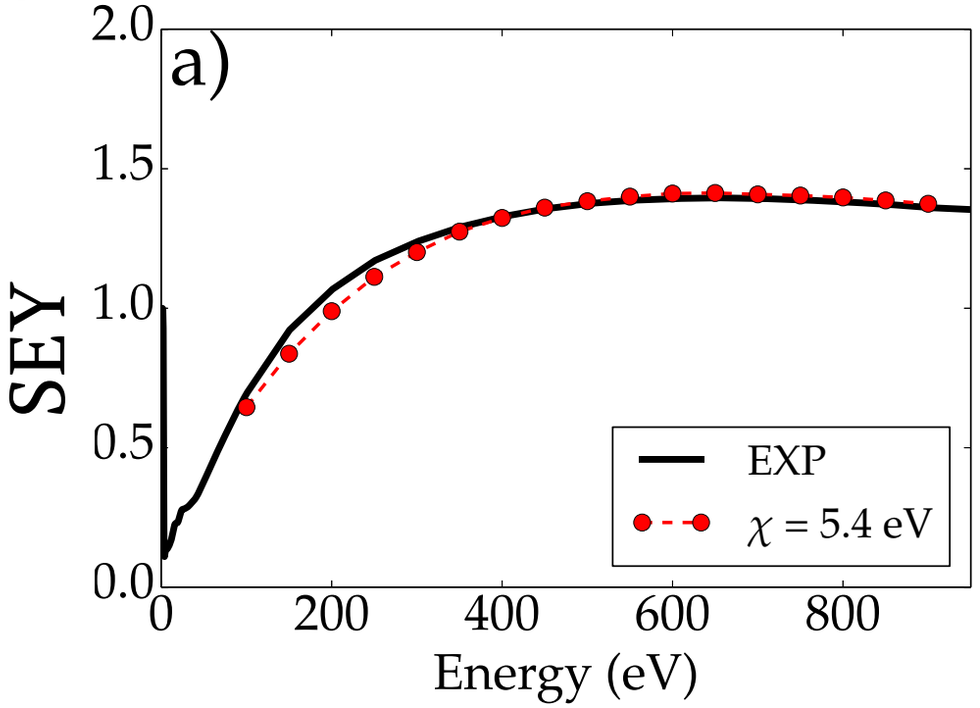
Secondary electron yield

$$\text{SEY} = \frac{\text{n° of emitted electrons}}{\text{n° of total trajectories}}$$

Simulation realized by considering 10^6 electrons in the beam

Copper



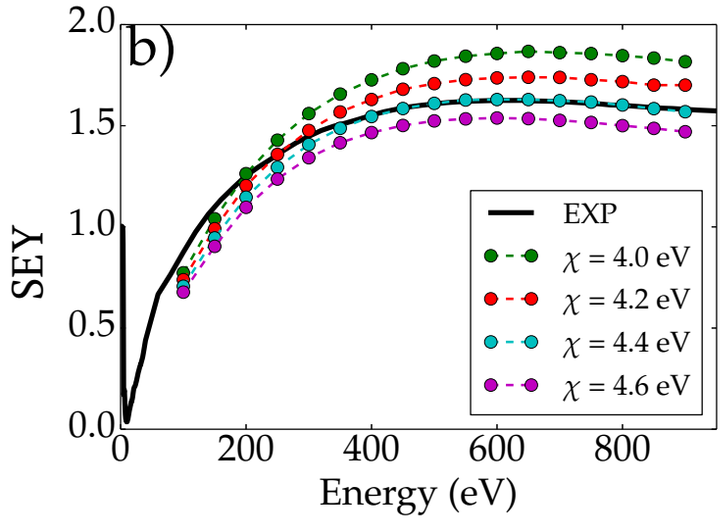


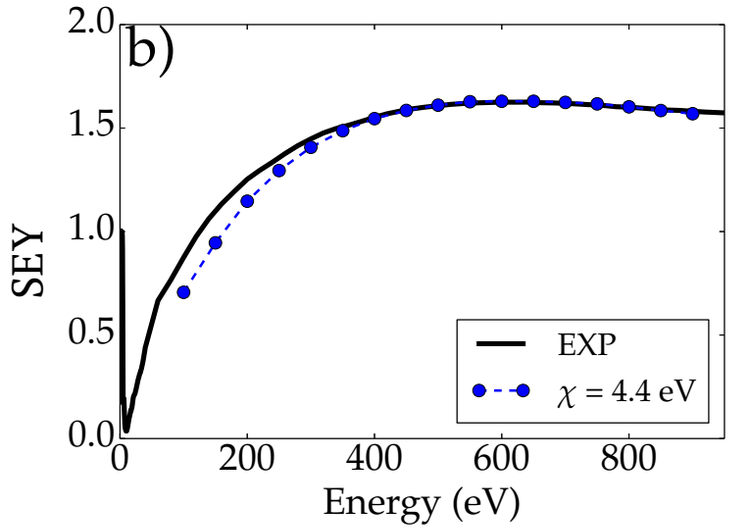
Experimental $\chi = 4.6$ eV

L. Gonzalez, M. Angelucci, R. Larciprete, R. Cimino, The secondary electron yield of noble metal surfaces, AIP Advances 7 (11) (2017) 115203.

Secondary electron yield

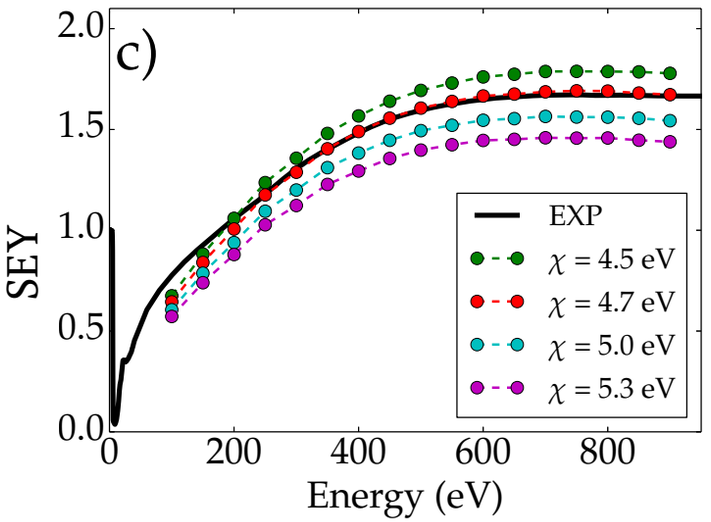
Silver

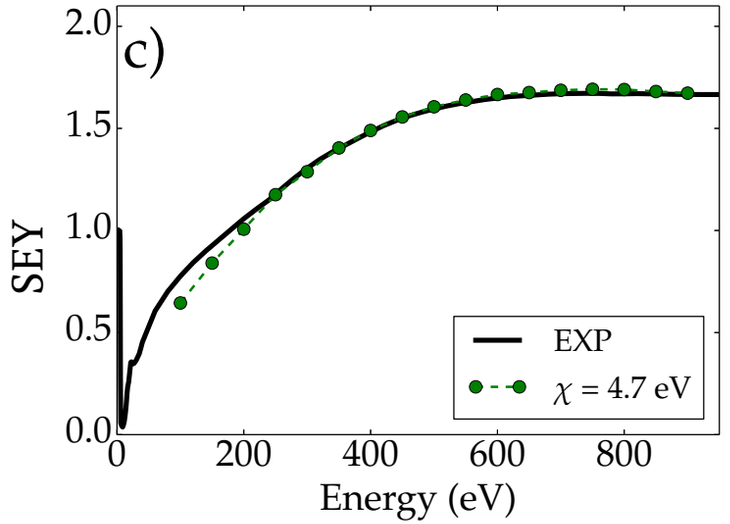




Experimental $\chi = 4.4$ eV

Gold





Experimental $\chi = 5.3$ eV

L. Gonzalez, M. Angelucci, R. Larciprete, R. Cimino, The secondary electron yield of noble metal surfaces, AIP Advances 7 (11) (2017) 115203.

Conclusions

- We developed a MC code to calculate electron trajectories in metal targets.
- The ionization and relative secondary electron generations are taken into account.
- Good agreement between calculations and experimental data of emission spectra and electron yield is obtained.

Next step

- Test the code by using energy loss function and secondary electron yield realized on the same sample.

Acknowledgements

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