Problems with low-energy electrons in imaging and lithography

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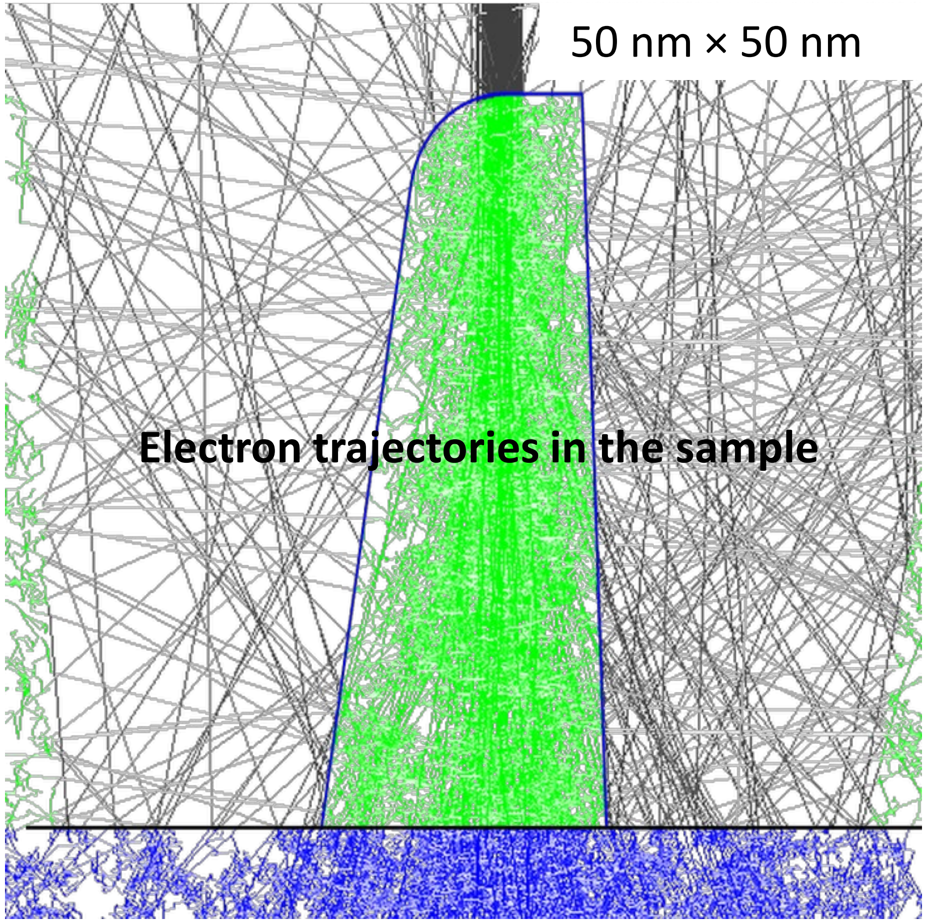
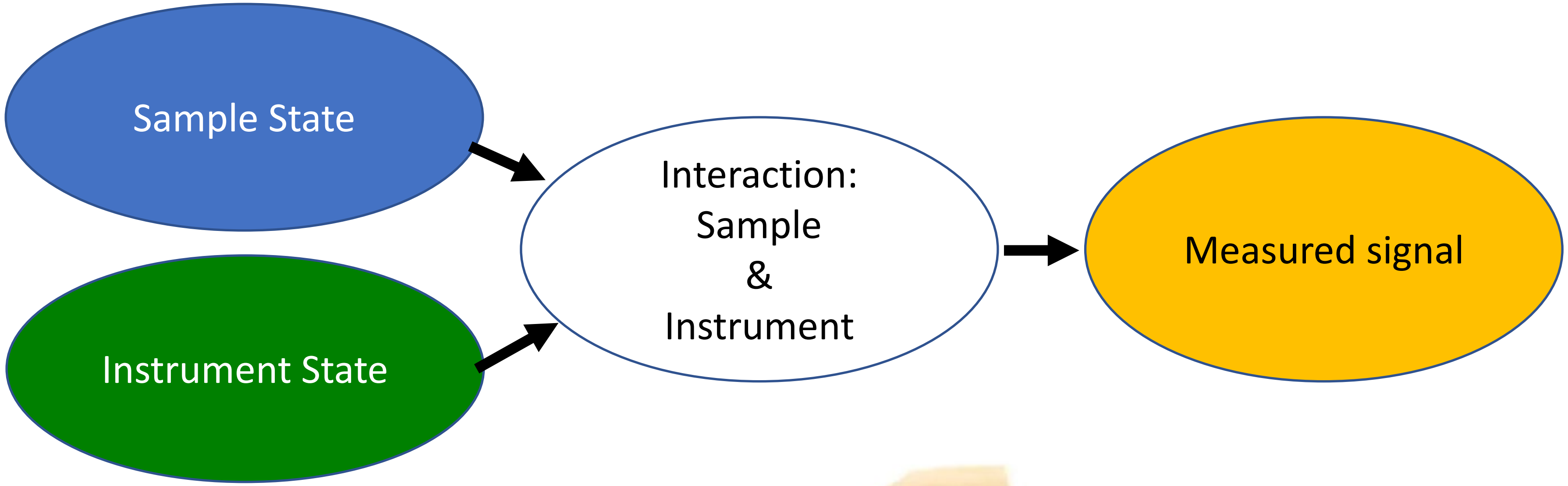
Scanning Electron Microscope



Measurement is science-based inference.



Sample State

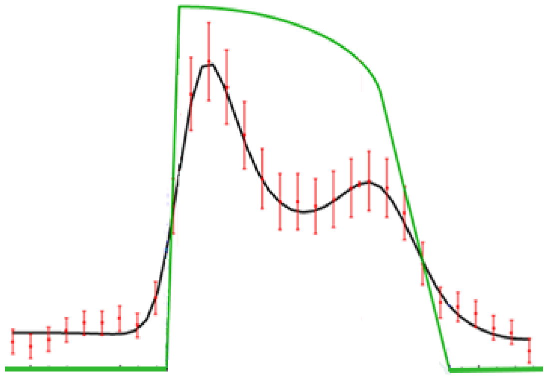
Instrument State

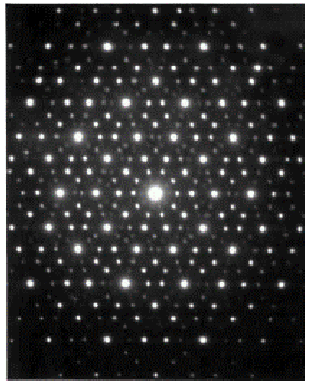
Interaction:
Sample
&
Instrument

Measured signal

Or mathematically

$$S(x,y) = f_M(x,y;s_i,I_j)$$



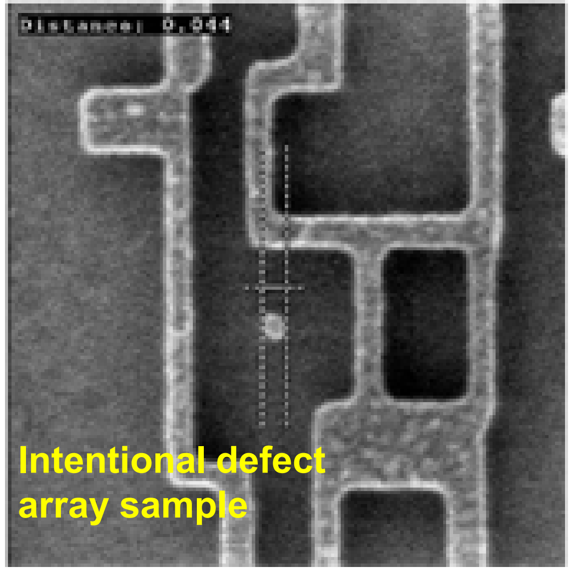


The models we use

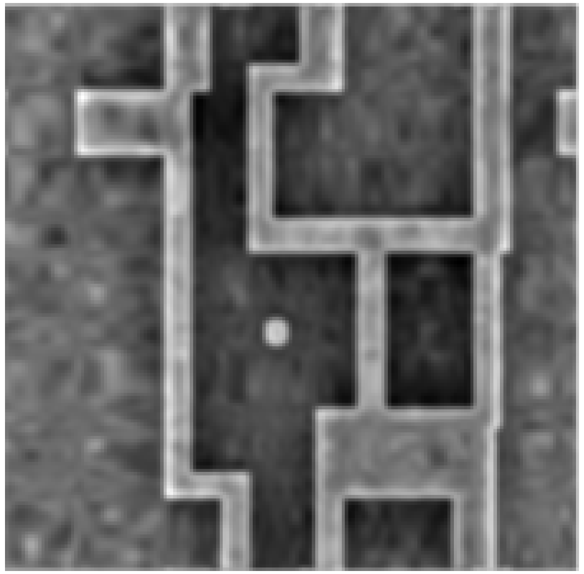
JMONSEL is a tool for measurement.

JMONSEL = “Java MONte Carlo Simulator for Secondary ELectrons”

It’s a tool to simulate SEM signals, including secondary electron contrast.



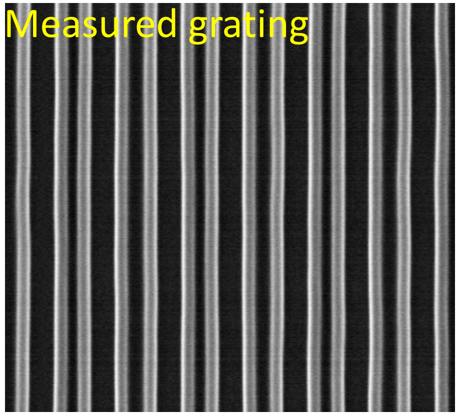
Secondary Electron Image

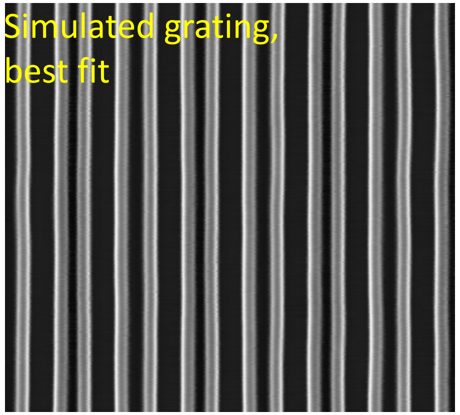


JMONSEL Simulation

- It’s meant to help us solve this problem: Given a measured image, $I(\boldsymbol{x})$, what was the shape, S, of the feature that produced it?

$$I(\boldsymbol{x}) = M(\boldsymbol{x}, S)$$



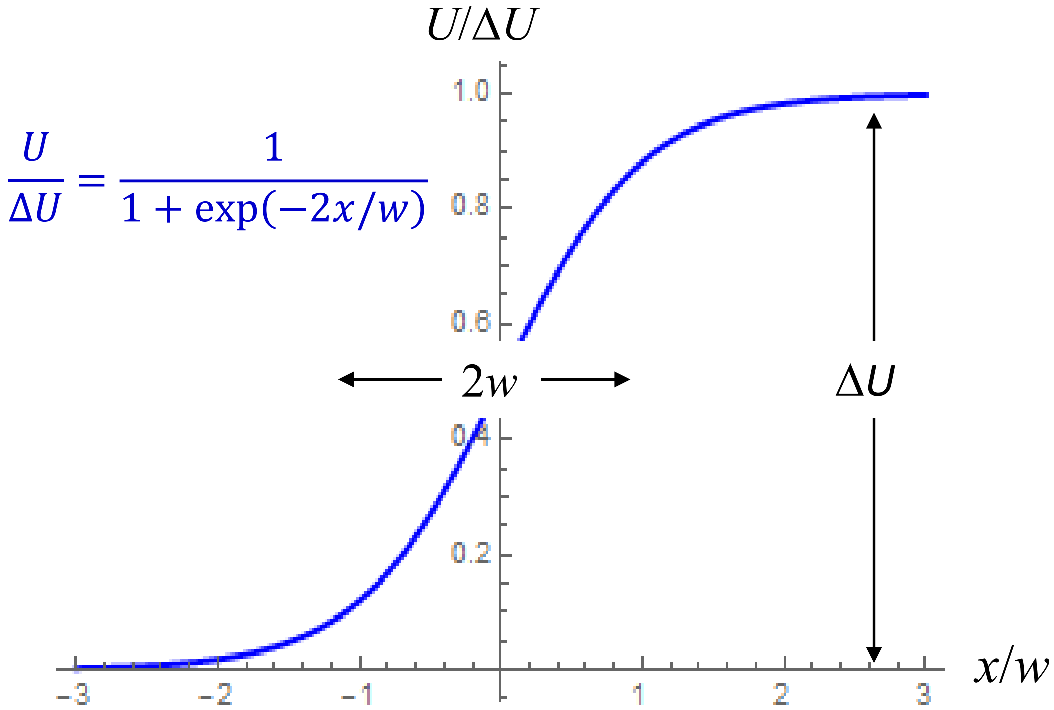


JMONSEL has models for…

- Boundary scattering at interfaces between materials
  - Quantum barrier with adjustable barrier width and height
- Electron-atom elastic scattering
  - Mott cross-sections in the relativistic partial wave method
- Electron-electron interactions in condensed materials
  - Dielectric function theory (Full Penn method)
- Electron-phonon scattering
  - Frölich's theory following the implementation of Lacer & Garwin, J. Appl. Phys. 40 (1965) 2766
- Electron-polaron trapping
  - Ganachaud & Mokrani, Surf. Sci. 334 (1995) 329
- It has alternatives to many of the above that can be used for comparison or for speed in appropriate circumstances.

Boundary scattering

An electron must "go uphill" to get out of the sample.
Sometimes it undergoes specular reflection.
Sometimes it transmits with refraction.



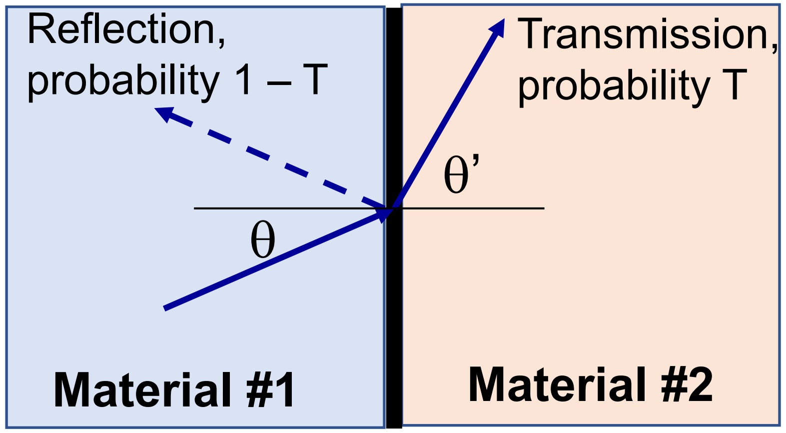
$$\frac{U}{\Delta U} = \frac{1}{1 + \exp(-2x/w)}$$

potential energy, U(x), with barrier at $x = 0$

We model an S-shaped barrier with
2 parameters: height & width.

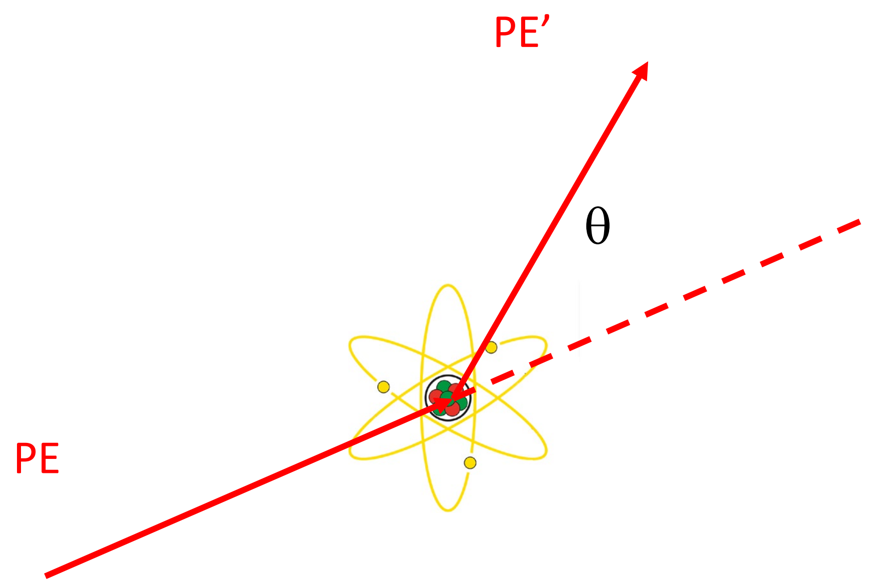
The quantum mechanical transmission probability is

$$T(E,\theta) = \begin{cases} 1 - \left(\dfrac{\sinh\left[\frac{1}{2}\pi w(k_1 - k_2)\right]}{\sinh\left[\frac{1}{2}\pi w(k_1 + k_2)\right]} \right)^2 & E\cos^2\theta > \Delta U \\ 0 & \text{otherwise} \end{cases}$$



Barrier scattering

Elastic scattering



Elastic scattering

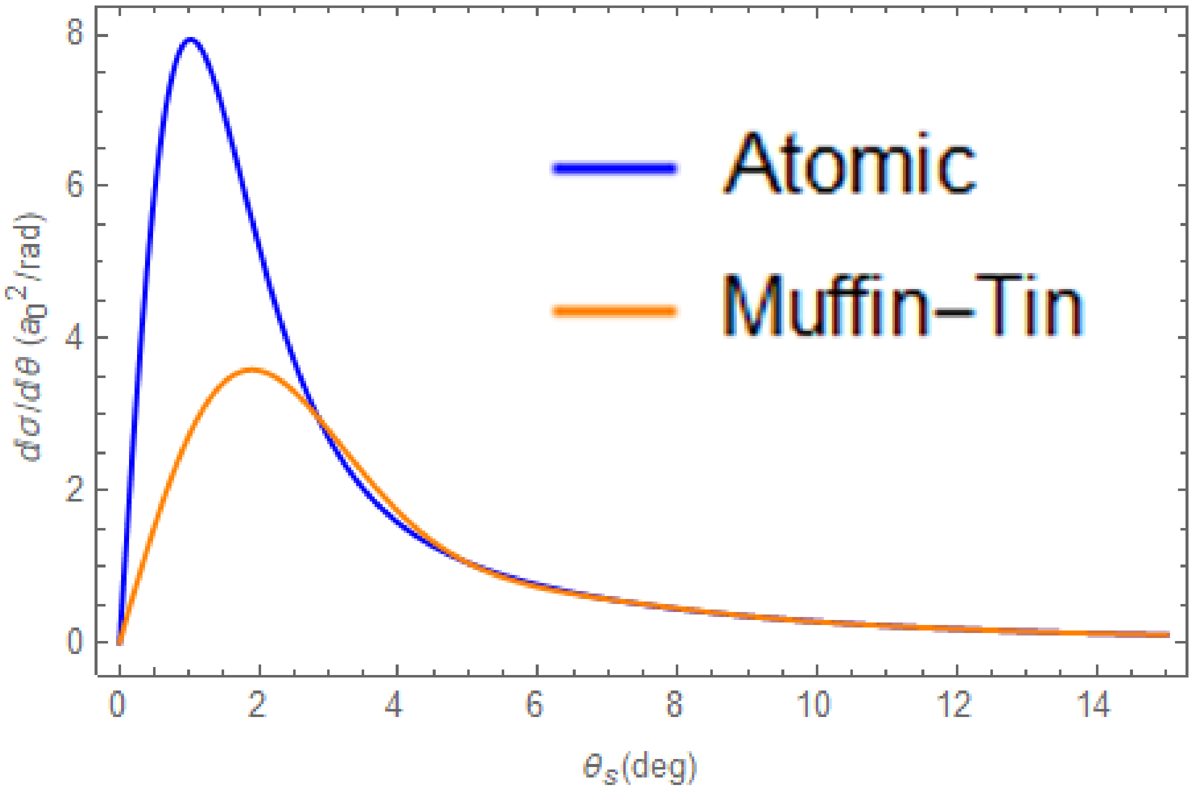
Collision with atom, no atomic excitation

Minimal energy loss, often large deflection

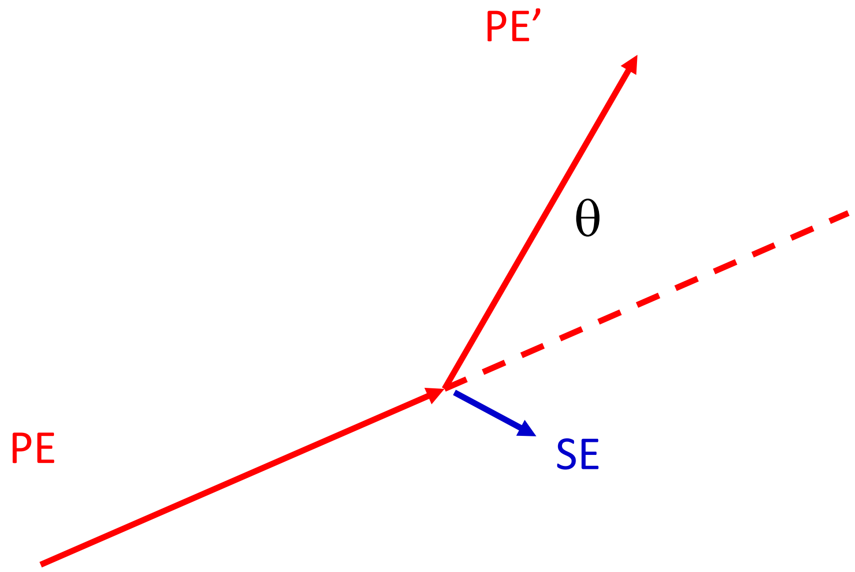
Elastic scattering model

- The state of the art for this is a relativistic partial wave analysis calculation of the Mott cross-sections with a detailed numerical approximation of the potentials inside the atoms.
- Luckily, F. Salvat has done this for us. There is a publicly available ELSEPA code that outputs $\frac{d\sigma}{d\Omega}$ at tabulated intervals. [F. Salvat et al., Comp. Phys. Comm. **165** (2005) p 157, updated **261** (2021) 107704]
- This code is the foundation for NIST SRD 64, a tabulation of scattering from atomic potentials.
- I’ve used it to generate scattering tables for both atomic and muffin-tin potentials for all the stable elements for use in JMONSEL.

Scattering cross section vs. angle
Si at 20 keV



Inelastic scattering, SE generation model



Inelastic scattering (SE generation)

Energy loss near 20 eV, small deflection

Inelastic scattering, SE generation model

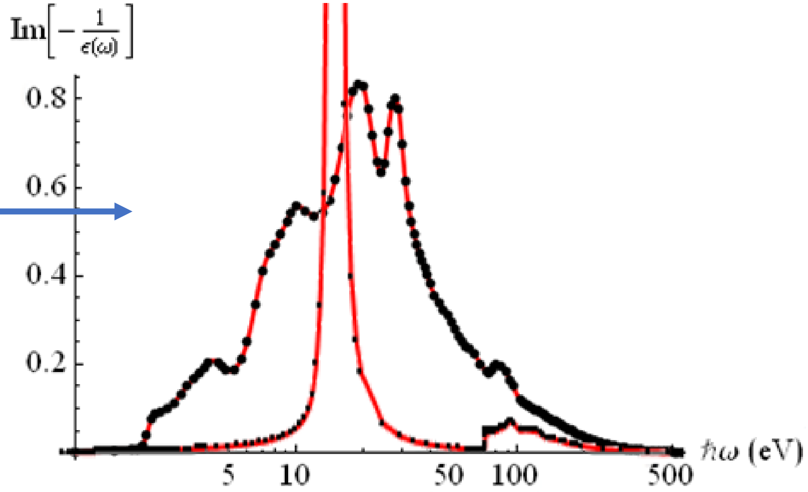
Energy loss function (ELF)

(In atomic units) $$\frac{d^2\lambda_{\text{in}}^{-1}}{d\omega\, dq} = \frac{2}{\pi\, v^2}\text{Im}\left[\frac{-1}{\varepsilon(q,\omega)}\right]\frac{1}{q}$$

This is the DIMFP of Pines & Nozières (1966)
v is the speed of the primary electron.

The ELF is usually not known. However, if our material were a free electron gas (FEG) with plasmon at ω_p, there is a theoretical relationship between $\text{Im}\left[\frac{-1}{\varepsilon(q=0,\omega;\omega_p)}\right]$ and $\text{Im}\left[\frac{-1}{\varepsilon(q,\omega;\omega_p)}\right]$ derived by Lindhard. We can use that for Al but not for Cu.

$q = 0$ Energy Loss Function



D.R. Penn [Phys. Rev. B 35 (1987) 482] proposed this integral transform:

$$\text{Im}\left[\frac{-1}{\varepsilon(q,\omega)}\right] = \int_0^\infty d\omega_p \frac{2}{\pi\omega}\text{Im}\left[\frac{-1}{\varepsilon(0,\omega)}\right]\text{Im}\left[\frac{-1}{\varepsilon^L(q,\omega;\omega_p)}\right]$$

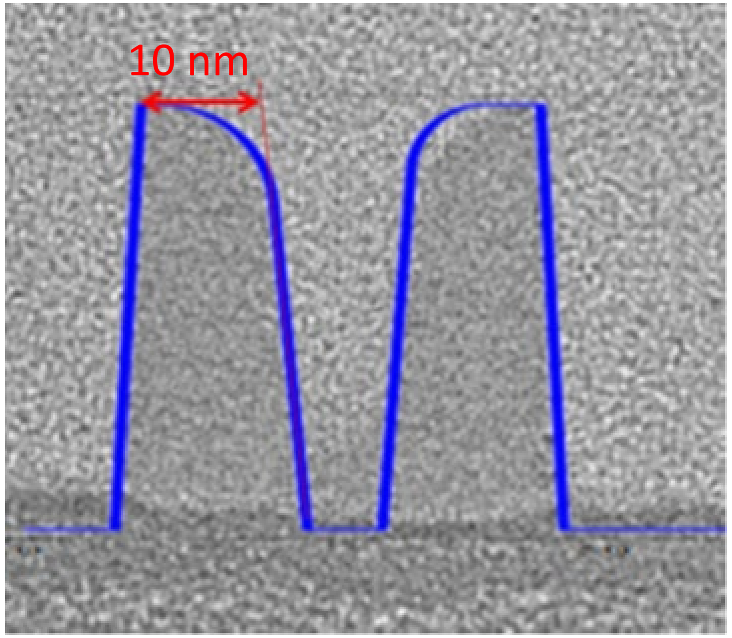
This is the *optical* ($q = 0$) energy loss function of the material. It is in principle measurable, e.g., at a synchrotron.

This is a known function, Lindhard's dielectric function for a FEG, and it is the *only* place q appears on this side of the equation.

Physics usually improves measurement accuracy

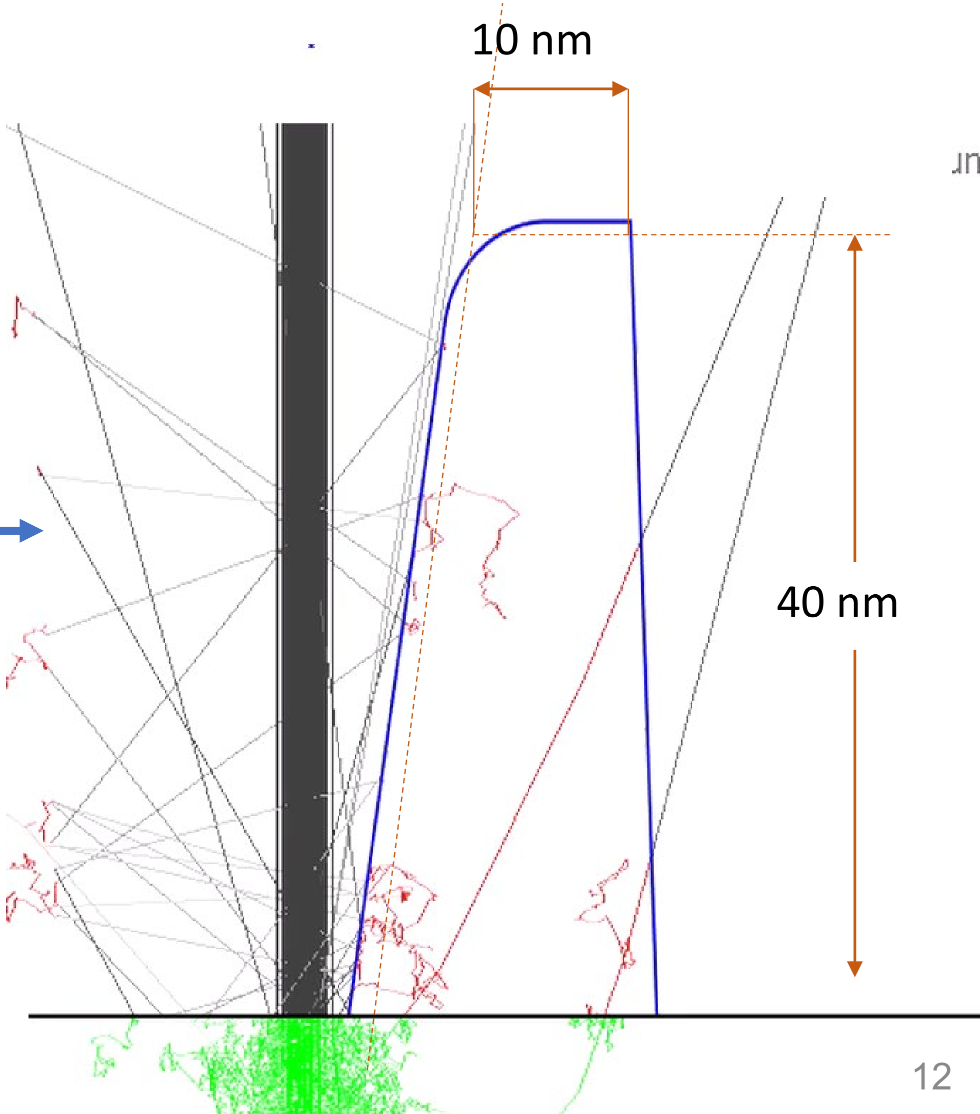
JMONSEL simulator calculates the expected signal for a given sample.

Simulated SEM line-scan of a “shark-fin” line with a 15 keV Gaussian ($\sigma = 1$ nm) electron beam.



Method	$w_{\text{mid}} \pm 2\sigma$ (nm)
MBL-SEM	13.4 ± 0.2
TEM	12.9 ± 0.3
CD-SAXS	12.6 ± 0.3

J. S. Villarrubia et al., Ultramicroscopy **154**, 15–28 (2015) [doi:10.1016/j.ultramic.2015.01.004]



Resulting simulated linescan

Scan simulation

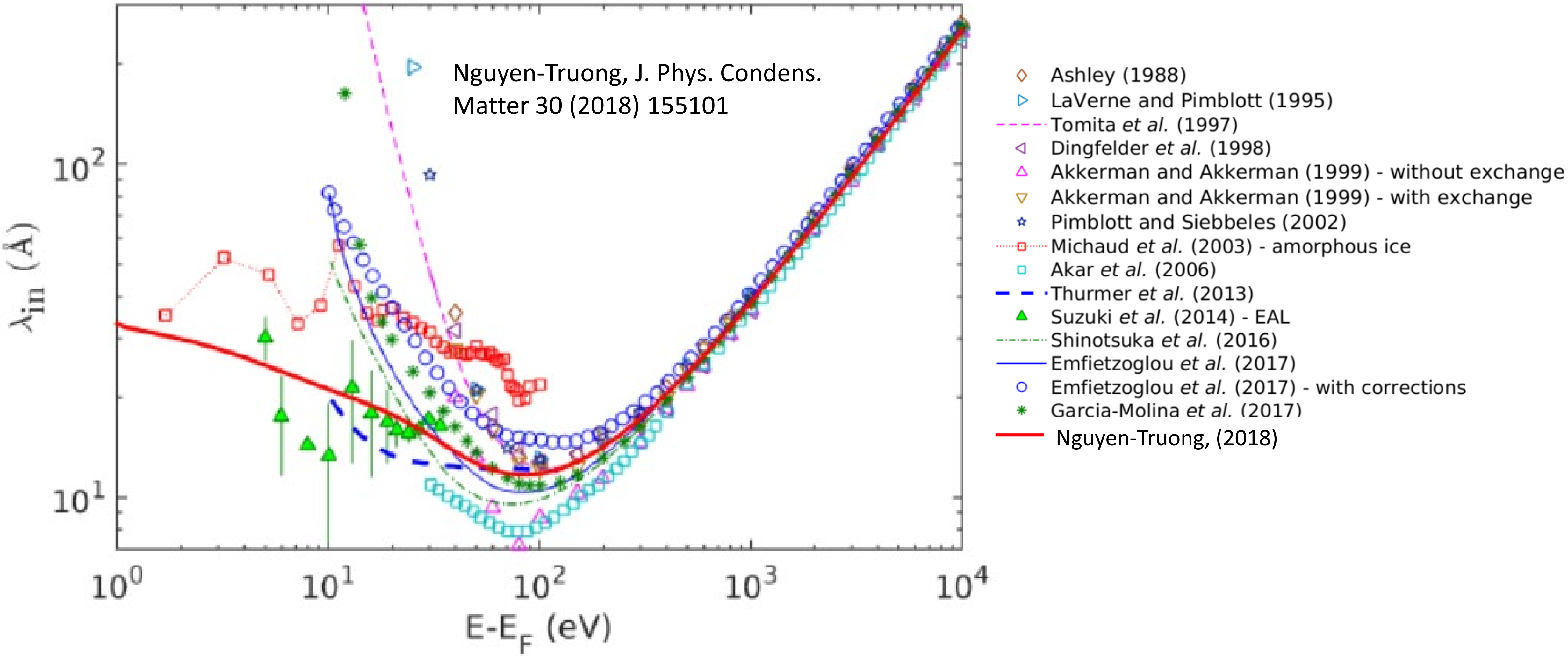
…but this is far too happy an ending to stop now…

If that were the whole story, what would we brainstorm about?

Some less auspicious signs:

- $w_{\mathrm{SEM}} - w_{\mathrm{CD-SAXS}} = 0.8 \pm 0.4$ nm (2σ). This difference is statistically significant. This means it's highly likely that there is a bias between these techniques.
- We should expect $\frac{\chi^2}{\nu} = 1$ with accounting for all uncertainties.
  - In fact, the MBL-SEM fit had $\frac{\chi^2}{\nu} = 1.26.$
  - This means there is "dark uncertainty" (error sources that have not been included in the uncertainty estimate—probably model errors).
- There are other reasons to question our models…

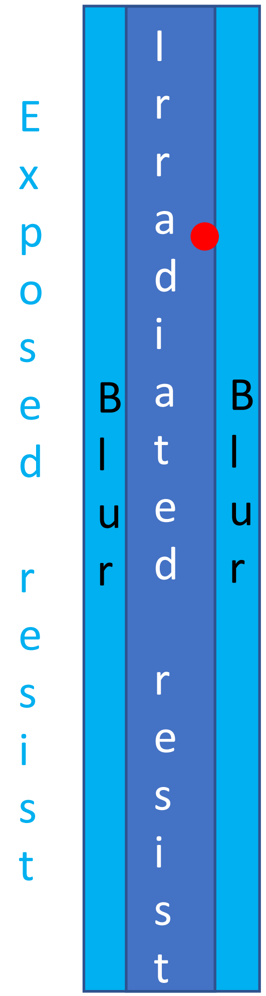
Mean free path models disagree at energies < 200 eV



Nguyen-Truong, J. Phys. Condens. Matter 30 (2018) 155101

Inelastic mean free paths in H_2O, different models

Lithography: electronic blur depends on very low energies.



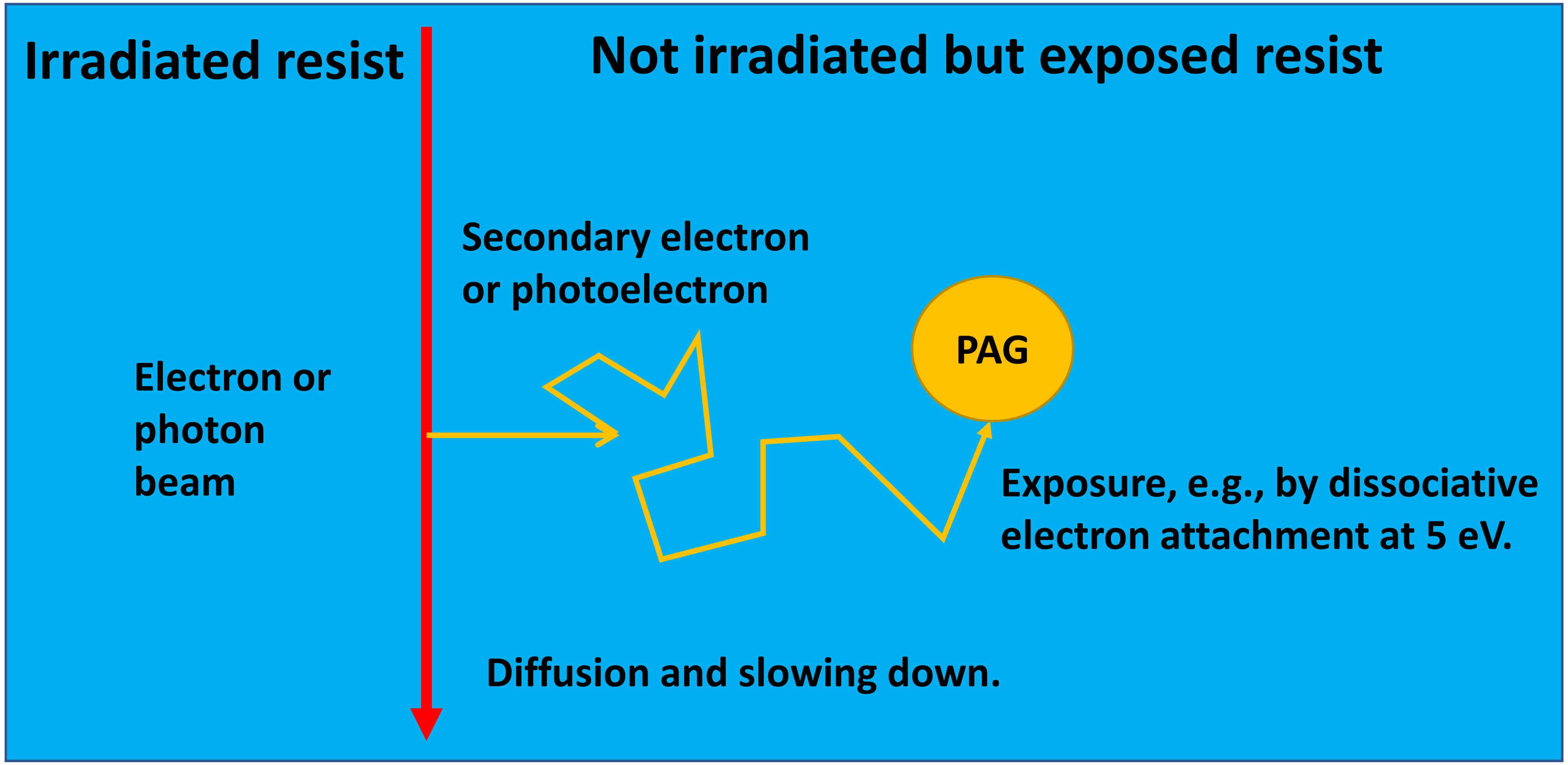
Exposed resist

Blur

Irradiated resist

Blur

Resist exposure extends beyond the intended boundaries.



Irradiated resist

Not irradiated but exposed resist

Electron or photon beam

Secondary electron or photoelectron

PAG

Exposure, e.g., by dissociative electron attachment at 5 eV.

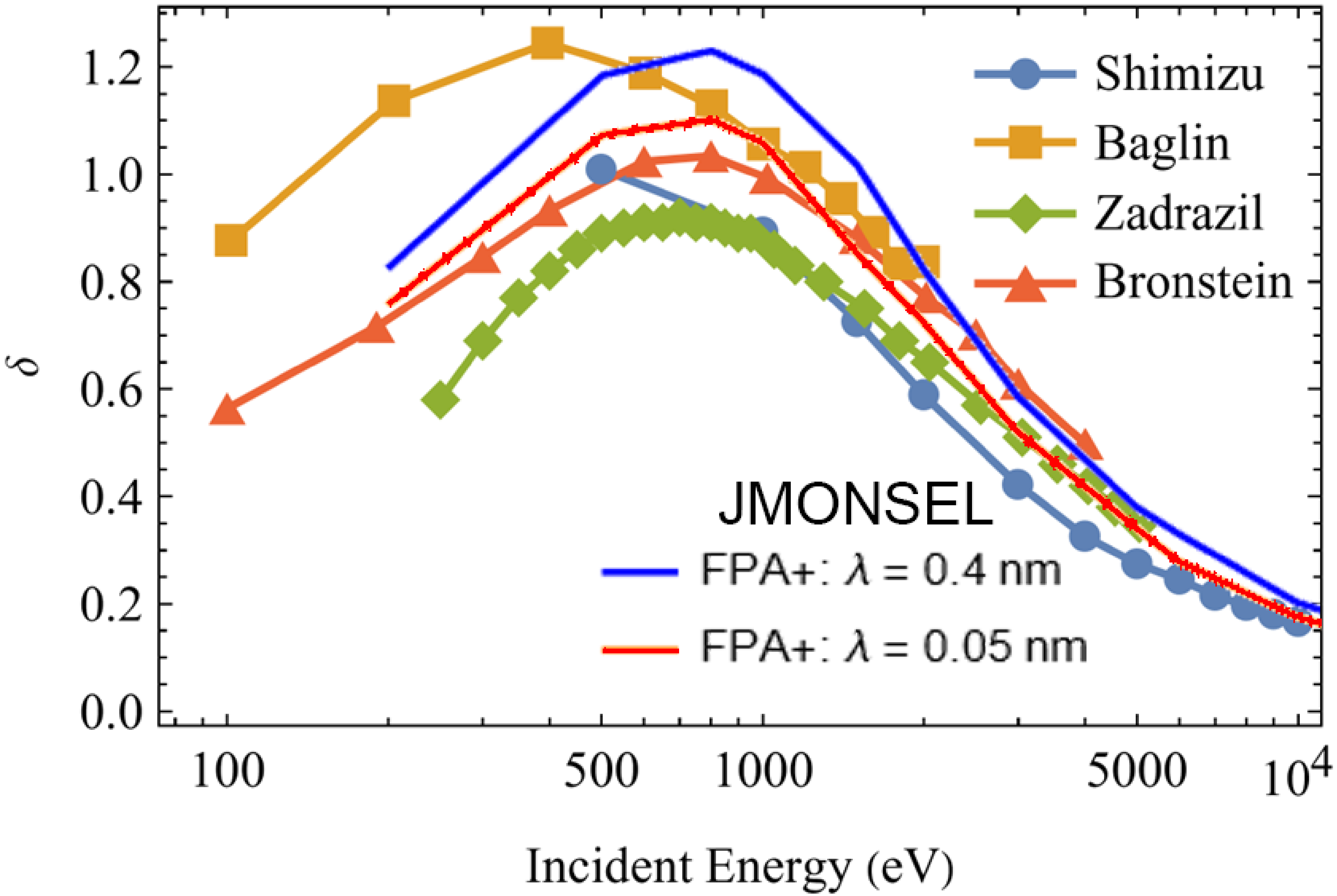
Diffusion and slowing down.

Lowest relevant energy:
For exposure—electron must be able to activate the exposure chemistry.
For imaging—electron must be able to escape the sample.

This may be a factor of 2 or 3 smaller than this.

Measured yields disagree. Measurements do not tell us which model is right.

Cu secondary electron yield measurements at different laboratories



Yield vs. tilt angle

Yield vs. surface slope is an important part of topographic contrast.

Most yield vs. angle measurements were taken years ago low energy SEM was less common. The measurements are at high energies.

Typical CD-SEM dimensional measurements are now done at 1 keV or lower. Departures from the "secant law" are more significant at such lower energies.

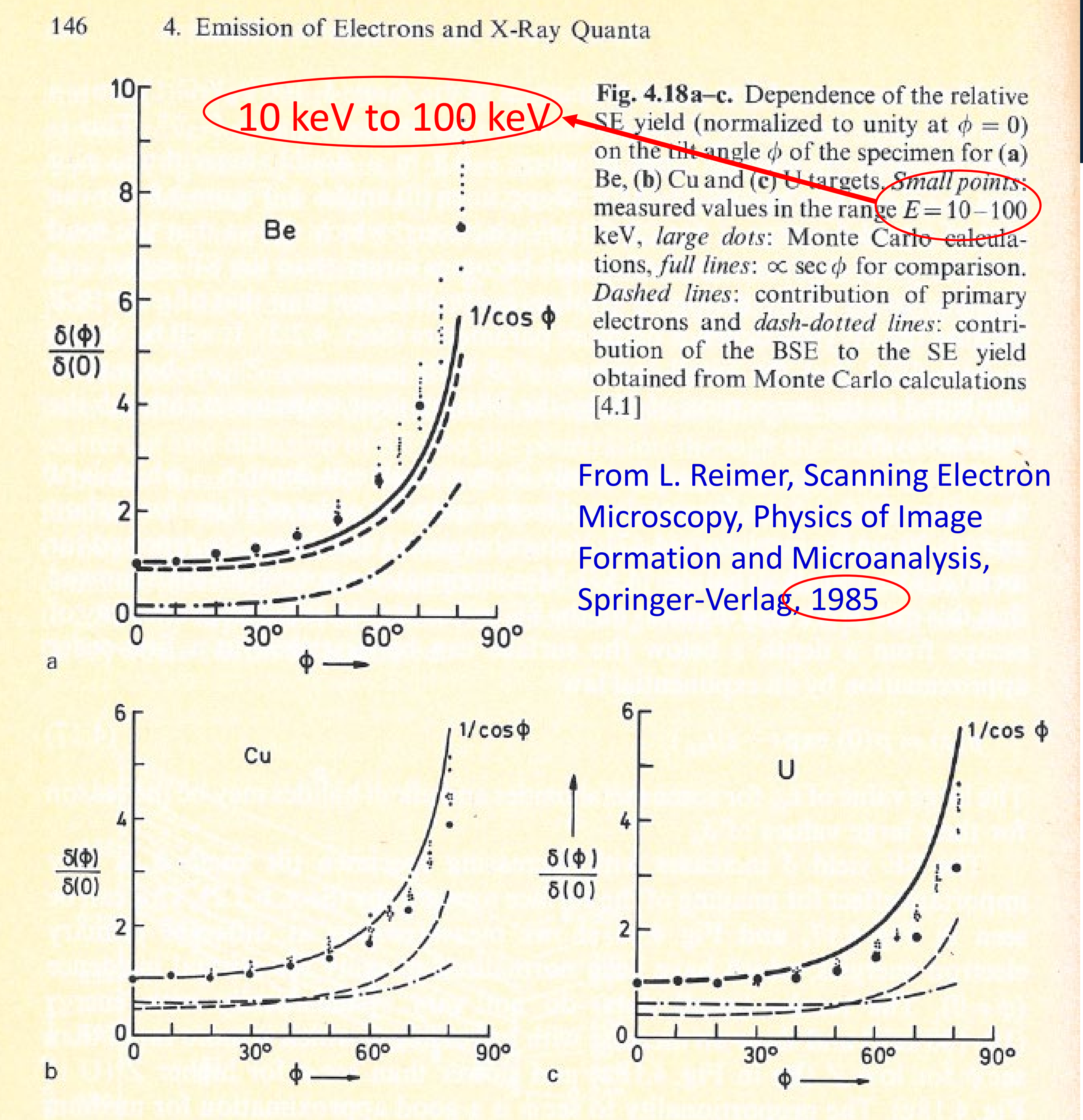


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Fig. 4.18a–c. Dependence of the relative SE yield (normalized to unity at $\phi = 0$) on the tilt angle ϕ of the specimen for (**a**) Be, (**b**) Cu and (**c**) U targets. *Small points*: measured values in the range $E = 10-100$ keV, *large dots*: Monte Carlo calculations, *full lines*: $\propto \sec\phi$ for comparison. *Dashed lines*: contribution of primary electrons and *dash-dotted lines*: contribution of the BSE to the SE yield obtained from Monte Carlo calculations [4.1]

10 keV to 100 keV

From L. Reimer, Scanning Electron Microscopy, Physics of Image Formation and Microanalysis, Springer-Verlag, 1985

Theoretical uncertainty: some of the approximations in our models

- The elastic scattering cross-sections from ELSEPA’s partial wave analysis are not recommended below 50 eV. Elastic scattering affects the diffusion path length of SE to the surface.
- The inelastic scattering model uses many high-energy approximations:
  - Born approximation used to derive the scattering cross section.
  - The random phase approximation.
- Dielectric function models mostly ignore quantum mechanical exchange and correlation.
- The superposition of free electron gas ELFs for $q > 0$
  - does not account for band structure effects
  - does not account for electron-hole interaction
  - is a theory of energy loss by the primary electron. Secondary electron energy and momentum require us to model initial energy and momentum.

Summary

Summary

- Model physics is an integral part of measurement at the nanometer scale.
  - We use physics to make a simulator that predicts the measured signal given the sample and instrument details.
  - I gave you a quick overview of the most important models we use.
  - When we find a sample geometry for which simulated image = measured image, we have a measurement.
  - Model errors lead to measurement errors
- Our measurements do quite well sometimes, but there are indications of model errors important for image interpretation and lithography.
- Existing measurement data have high variability so don’t sufficiently constrain our choice of model.

My project needs a new postdoc/guest researcher

Experimental project: Electron microscopy—imaging physics—instrument characterization

Send your CV or questions to semmod@nist.gov