Nebula: Monte Carlo simulator of electron-matter interaction



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The interaction of 0–50 keV electrons with matter is of great interest in nanofabrication. Scanning electron microscopes (SEMs) are used by the semiconductor industry to monitor process parameters such as critical dimension and line-edge roughness (LER). As device features shrink below 20 nm, the image formation process in SEMs becomes increasingly important. In addition, the electron cascade in resist defines the pattern shape in both electron-beam lithography and extreme ultraviolet lithography. Furthermore, electron-beam induced patterning is a technique for high-resolution patterning within an SEM. Slow electrons emitted from the substrate dissociate precursor gas molecules to induce deposition or etching, which can be used to grow 3D structures.

Nebula is an open-source Monte Carlo package to simulate such electron-matter interaction.

https://nebula-simulator.github.io

It's fast

Comparable simulators often take hours to simulate a single SEM image. Empirical physical models are sometimes used to make them faster. Nebula runs on graphics cards (GPUs), which makes it orders of magnitude faster while using fully physical models.

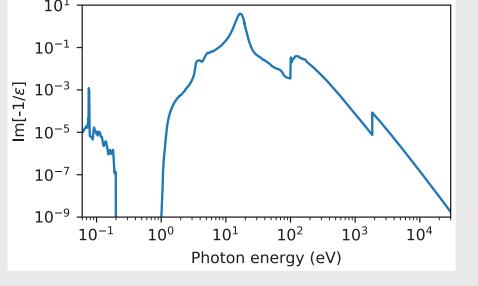
Beam energy	Single-thread CPU [1]	GPU [2]	Speedup
5 keV		32m	894×
3 keV	Iw 4d 20h	22m	796×
I keV	3d IIh	I0m	538×
800 eV	2d 17h	8m	530×
500 eV	ld I0h	5m	472×
300 eV	15h 16m	3m	387×
Beam energy	10-core CPU [3]	GPU	Speedup
3 keV	2h	90s	80 ×

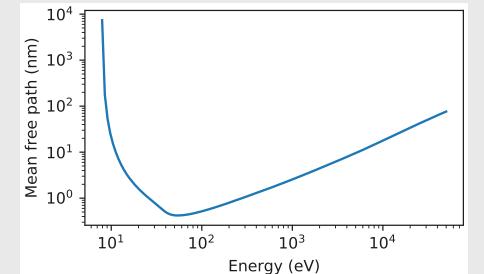
- [1] Kieft et al. J. Phys. D 41 (2008) 215310
- [2] Verduin et al. Proc. SPIE 9778 (2016) 97780D
- [3] Zou et al. Measurement 123 (2018) 150-162

Inelastic scattering

In an inelastic event, an electron loses energy. A secondary electron may be excited from the material.

We use the material's measured dielectric function, and fit it to a free-electron gas model describing valence electrons, to describe inelastic scattering.

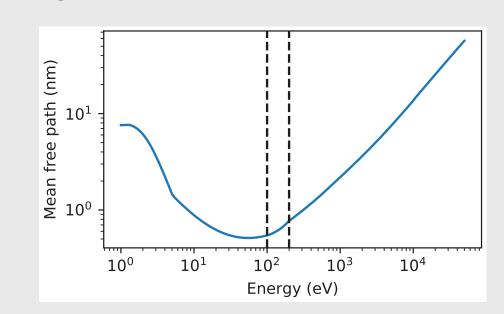




Elastic scattering

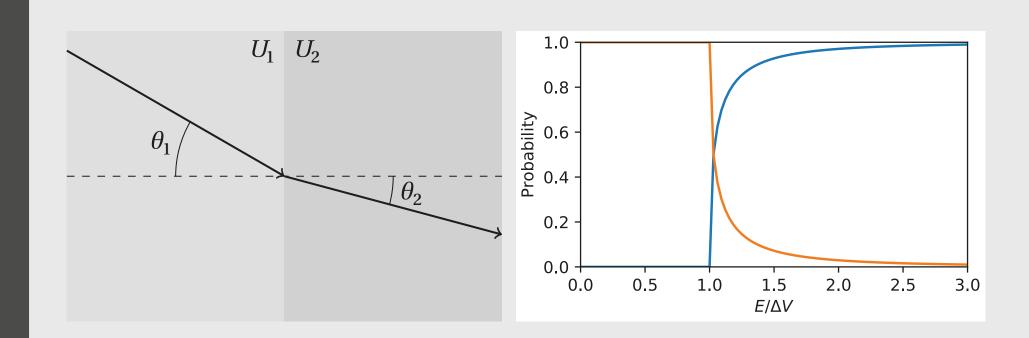
In an elastic event, an electron is deflected without losing energy.

We describe this by Mott scattering at high (> 200 eV) energies, and by electron-phonon scattering at low (<100 eV) energies.



Boundary crossing

When an an electron crosses a material boundary, it sees a local potential change due to the difference in work function. The electron may change direction (similar to refraction of light), or it may be specularly reflected if its energy is low.



3D sidewall roughness in line-edge roughness measurements

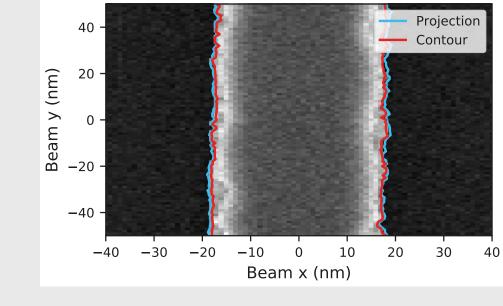
Line-edge roughness (LER) is often measured from top-down SEM images. The true three-dimensional roughness profile of the sidewall is typically ignored in such analyses.

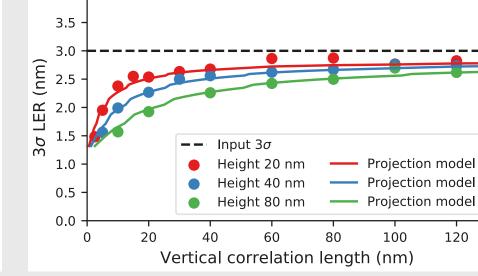
We generated random rough lines and spaces, with sidewall roughness (SWR) modelled by a known power spectral density. We then obtain corresponding SEM images using Nebula. We measure LER in these images and compare it to the input roughness.

When a line is isolated (no neighbours), the "projection model" describes the measured LER very well.

A SEM image is bright when the electron beam lands near a sharp edge. The same happens when the beam lands on an extrusion on the rough sidewall. The SEM contour then goes around all

extrusions as seen from the top. The measured LER is less than the true SWR as a result.

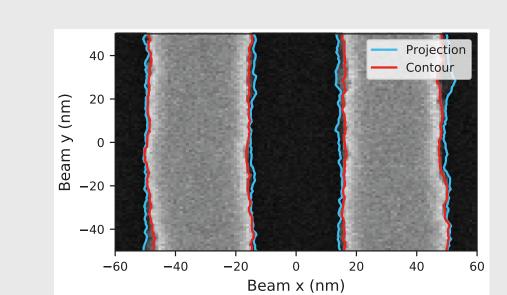


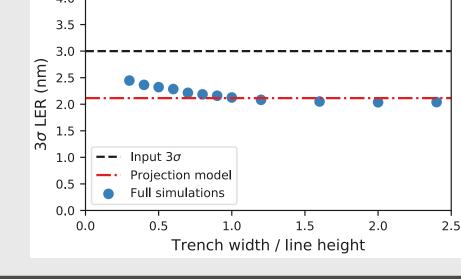


For dense lines & spaces, electrons escaping from lower layers of the structure are blocked by neighbouring lines.

As a result, deeper layers are darker in the SEM image. The projection model fails when this effect becomes too strong, but it is quite accurate when the line height is less than the trench width.

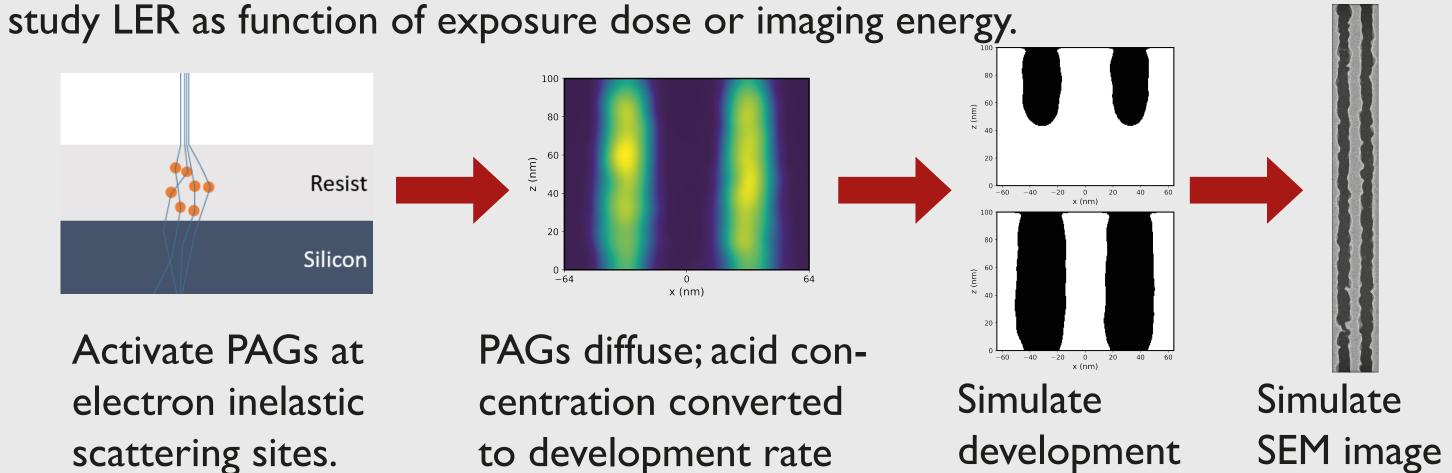
[1] Van Kessel et al. J. Micro/Nanolith. MEMS MOEMS 19 (2020) 034002





Electron beam lithography

We can simulate a full electron-beam lithography workflow. We use Nebula to define where photoacid generators (PAGs) are activated. With a development model, we obtain a final 3D profile. We then simulate a SEM image. This can e.g. be used to



Electron beam induced deposition

In electron-beam induced deposition, a precursor gas is injected near a substrate. When illuminated by an electron beam, the molecules are dissociated and fragments stick to the surface. We can simulate this process, track growth through time and discover which electrons are most likely to contribute to deposition.

