

## An accurate Monte Carlo sampler for electron elastic scattering angular distributions between 50 eV and 300 keV

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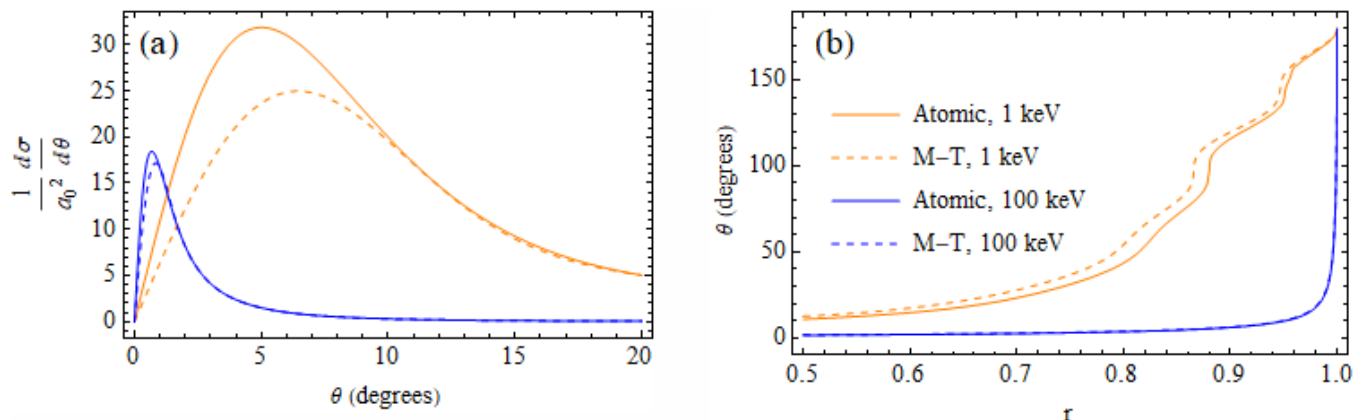
Elastic scattering of electrons is an important determiner of the signal in many sensitive analytical measurement techniques, including scanning or transmission electron microscopy (SEM, STEM, or TEM), Auger electron spectroscopy, photoelectron spectroscopy, and x-ray microanalysis, among others. Signals from these instruments may be predicted or interpreted with the help of Monte Carlo electron transport simulators. In Monte Carlo simulators, a “sampler” is a function that accepts an easily available random number (e.g., uniformly distributed in  $[0,1]$ ) as input and returns a random value drawn from another desired distribution. For example, if  $\theta$  is the scattering angle in an elastic collision between an electron and an atom, we may wish  $\theta(E,r)$  to reproduce for electrons of energy  $E$  the distribution of scattering angles predicted by Dirac partial-wave theory, e.g., as provided by ELSEPA.<sup>1,2</sup> ELSEPA calculations provide the values for version 3.2 of NIST’s standard reference database 64 (SRD 64),<sup>3</sup> which provides tabulations of samplers using ELSEPA’s default model for elements with  $Z = 1$  to  $Z = 96$ . The samplers are tabulated at 60 logarithmically uniform intervals for energies in  $[50 \text{ eV}, 20 \text{ keV}]$  and intervals in  $r$  from 0 to 1 in steps of 0.005.

Uniformly spaced tables are easy to interpolate, but the interval size limits the maximum energy of the tables, as illustrated in Fig. 1. As the electron energy increases, scattering by less than one or a few degrees accounts for an increasing fraction of the differential cross section (DCS, Fig. 1a). E.g., for Au at 100 keV, 99 % of events have  $q < 28^\circ$ . This means in the sampler (Fig. 1b), events for the remaining angles,  $28^\circ < \theta < 180^\circ$ , are confined to the narrow and sparsely sampled peak with  $0.99 < r < 1$ . Though these large angle events are rare, they contribute disproportionately to STEM contrast (they are the ones that miss the bright field detector) or to backscattering yield in the SEM. It was for this reason that SRD 64 established its 20 keV cutoff.

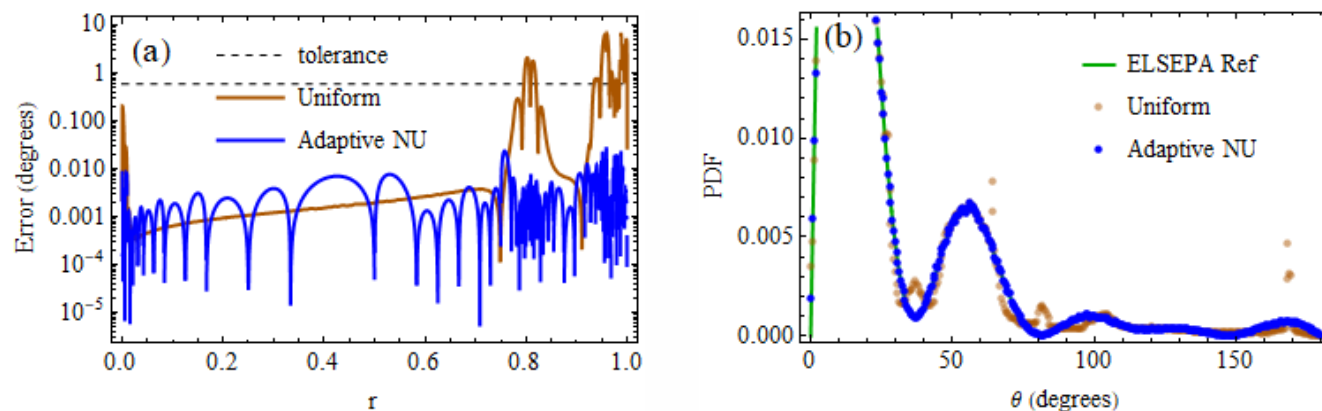
I have computed new samplers for JMONSEL<sup>4</sup> (our Monte Carlo electron transport simulator). The new tables use ELSEPA atomic and muffin-tin models, but the functions are sampled adaptively and at unequal intervals for energies from 50 eV to 300 keV. For a given energy, ELSEPA first generates a densely sampled DCS. A high-accuracy “reference sampler” is computed from the DCS in mathematical software with an adaptive numerical differential equation solver. The reference sampler is tabulated iteratively, starting with a uniform but coarse sampling. Cubic interpolation of the tabulated values is compared to the reference function at  $1/4$ ,  $1/2$ , and  $3/4$  of the interval. If the difference exceeds tolerance, a new sample is added at mid-interval. The iteration stops when interpolation of the table agrees with the reference sampler to within tolerance in all intervals. This is repeated at other energies. These are likewise initially coarsely sampled with new samples added as needed until convergence.

The tolerance condition required the angular error to be smaller than  $0.1^\circ$  or 3% of the forward scattering peak’s full width at half maximum, whichever is larger. A second tolerance required the energy sampling to be such that error in the interpolated total cross section be less than 0.5%. With these tolerances the new tables required samples at only 47 % as many  $(E,r)$  pairs as did the uniformly sampled tables. This is remarkable given that they must span an energy range 15 times larger.

An example of the performance of the adaptive non-uniform (NU) sampler relative to the previous uniform sampler is shown in Fig. 2. At an energy close to mid-energy-interval for both (where errors are expected to be high) the error as a function of  $r$  is shown in Fig. 2a. The adapted version's errors are more even and are within tolerance. The uniformly interpolated version is well within tolerance over most of the  $r$  range, but exceeds tolerance by as much as a factor of 7 at high  $r$ , where denser sampling was needed. The effect of these errors on the distribution of sampled  $\theta$  values is shown in Fig. 2b. There, histograms of  $10^6$   $\theta$  values for each of the samplers are compared to the reference probability distribution function from ELSEPA. Differences are observed mainly at the bottom of the scale, i.e., for low probability events. These are unlikely to be important except under very unusual circumstances. The main advantage of the adaptive interpolation is that it permits extending the energy range of the tables to 300 keV with a gain in accuracy for high-deflection events.



**Figure 1.** (a) The forward scattering peaks in the DCS (units of Bohr radius squared) of Au for 1 keV and 100 keV electrons in atomic and muffin-tin (M-T) models. (b) The corresponding sampler functions,  $\theta(r)$  with  $r$  a random number uniform in the interval  $[0,1]$ . The legend serves for both (a) and (b).



**Figure 2.** (a) Interpolation errors relative to an ELSEPA reference for  $q(r)$  for 235 eV electrons incident on Au. (b) The corresponding normalized histograms of scattering angles for 106 random  $r$  values.

## References

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2. F. Salvat, A. Jablonski, and C.J. Powell, *Comput. Phys. Commun* **261** (2021) 107704.
3. A. Jablonski, F. Salvat, C. J. Powell, and A. Y. Lee, NIST Electron Elastic-Scattering CrossSection Database - Version 3.2, National Institute of Standards and Technology, Gaithersburg, MD (2016); <http://www.nist.gov/srd/database-64-32/>, retrieved 25 Feb. 2021.
4. J. Villarrubia et al., *Ultramicrosc.* **154** (2015) 15.