# Monte Carlo simulation of bremsstrahlung emission by electrons

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An algorithm for the simulation of bremsstrahlung emission by fast electrons using numerical cross sections is described. It is based on natural factorization of the double-differential cross section and on the fact that the intrinsic angular distribution of photons with a given energy can be very closely approximated by a Lorentz-boosted dipole distribution. The parameters of this angular distribution vary smoothly with the atomic number of the target atom and with the energies of the projectile's electron and the photon emitted. Results from simulations of thick-target bremsstrahlung are compared with experimental data. © *2002 American Institute of Physics.*
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An accurate description of the continuous background in x-ray spectra from samples irradiated by electron beams is of interest for quantitative electron probe microanalysis (EPMA), for the characterization of medical and analytical x-ray sources, for the dosimetry of high-energy electron beams and, in general, for studies of high-energy radiation transport. Monte Carlo simulation of electron–photon showers has become the fundamental tool used for these studies, and a number of general-purpose Monte Carlo codes are widely available.[1] The most advanced ones generate the photon energy from the ''scaled'' differential cross sections (DCS) compiled by Seltzer and Berger[2] which represent the state of the art in theoretical high-energy bremsstrahlung calculations. However, all of these codes determine the direction of the photons emitted from very rough approximations, in spite of the fact that intrinsic angular distributions (''shape functions'') consistent with the scaled DCS have been available for a long time. The difficulty is the enormous size of the numerical database needed to define the DCS as a function of the electron energy $E$, the photon energy $W$ and the direction of emission $\theta$. It has been claimed that using inaccurate shape functions is not a serious problem for thick targets, because a parallel electron beam is rapidly randomized by multiple elastic scattering and this ''washes out'' the intrinsic angular distribution, which would then be relevant only for thin samples. This is not true for the tip (high-energy part) of thick-target spectra, which arises from photons emitted in the early stages of beam penetration and, therefore, is still sensitive to the intrinsic angular distribution. In this letter we describe a simple and accurate method by which to simulate bremsstrahlung emission using the most accurate shape functions available at present.

We consider the bremsstrahlung DCS for electrons of energy $E$ in a low-density, amorphous, single element medium of atomic number $Z$. After integrating over the angular deflection of the projectile, the DCS depends only on the energy $W$ of the photon and the direction of emission, represented by the polar angle $\theta$ relative to the direction of the projectile, and can be expressed as

$$\frac{d^2\sigma}{dW\, d(\cos\theta)} = \frac{d\sigma}{dW}\, p(Z,E,\kappa;\cos\theta), \tag{1}$$

where $\kappa \equiv W/E$ is the reduced energy of the photon, $\mathrm{d}\sigma/\mathrm{d}W$ is the energy-loss DCS differential only in the energy of the emitted photon and $p(Z,E,\kappa;\cos\theta)$ is the shape function, i.e., the probability distribution function (PDF) of $\cos\theta$ for given values of $E$, $Z$ and $\kappa$ (normalized to unity). The scaled DCS is normally defined as $(\beta^2/Z^2)W\mathrm{d}\sigma/\mathrm{d}W$, where $\beta = v/c$ is the velocity of the electron in units of speed of light. Seltzer and Berger[2,3] produced extensive tables of the scaled DCS for all the elements ($Z=1-92$) and for electron energies from 1 keV to 10 GeV, which constitutes the most reliable theoretical representation of bremsstrahlung energy spectra available at present.

Numerical values of the shape function, calculated by partial-wave methods, have been published by Kissel *et al.*[4] for 144 benchmark cases. These authors also gave a parameterization of the shape function in terms of Legendre polynomials. Unfortunately, their analytical form is not suited to random sampling of the photon direction.

In previous simulation studies of x-ray emission from solids bombarded by electron beams,[5] the angular distribution of bremsstrahlung photons was described by semiempirical analytical formulas derived by Kirkpatrick and Wiedmann[6] (and subsequently modified by Statham[7]). The shape function obtained from the Kirkpatrick–Wiedmann–Statham (KWS) fit is

$$p^{(\mathrm{KWS})}(Z,E,\kappa;\cos\theta) = \frac{\sigma_x(1-\cos^2\theta)+\sigma_y(1+\cos^2\theta)}{(1-\beta\cos\theta)^2}, \tag{2}$$

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where the quantities $\sigma_x$ and $\sigma_y$ are independent of $\theta$. Although this simple formula predicts the global trends of the partial-wave shape functions of Kissel *et al.*[4] in certain energy and atomic number ranges, its accuracy is not sufficient for general-purpose simulations. In a preliminary analysis, we tried to improve the accuracy of this formula by determining the parameters $\sigma_x$ and $\sigma_y$ by directly fitting the numerical partial-wave shape functions, but the improvement was not significant. However, that analysis confirmed that the analytical form, Eq. (2), is flexible enough to approximate the ''true'' (partial-wave) shape, and it can be adapted even for projectiles with relatively high energies, say, with $E$ larger than $\sim$1 MeV, for which the angular distribution of emitted photons is peaked at forward directions.

The simulation method presented here is based on the following classical argument (see, e.g., the work of Jackson[8]). Assume that the incident electron is moving in the direction of the $z$ axis of a reference frame K at rest with respect to the laboratory frame. Let $(\theta', \phi')$ denote the polar and azimuthal angles of the direction of the emitted photon in a reference frame K$'$ that moves with the electron and whose axes are parallel to those of K. In $K'$, we expect that the angular distribution of the photons emitted will not depart much from the isotropic distribution.[8] Therefore, we consider the following ansatz for the shape function in K$'$:

$$p_{\mathrm{d}}(\cos\theta') = A\tfrac{3}{8}(1+\cos^2\theta') + (1-A)\tfrac{4}{3}(1-\cos^2\theta'), \quad (0 \leqslant A \leqslant 1), \tag{3}$$

which is motivated by the relative success of the KWS formula at low energies. The direction of emission $(\theta, \phi)$ in K is obtained by means of the Lorentz transformation,

$$\cos\theta = \frac{\cos\theta' + \beta}{1+\beta\cos\theta'}, \quad \phi = \phi'. \tag{4}$$

Thus, the angular distribution in K is

$$p(\cos\theta) = A\frac{3}{8}\left[1+\left(\frac{\cos\theta-\beta'}{1-\beta'\cos\theta}\right)^2\right]\frac{1-\beta'^2}{(1-\beta'\cos\theta)^2} + (1-A)\frac{4}{3}\left[1-\left(\frac{\cos\theta-\beta'}{1-\beta'\cos\theta}\right)^2\right] \times \frac{1-\beta'^2}{(1-\beta'\cos\theta)^2}, \tag{5}$$

with $\beta' = \beta$. Now, it is clear that when $\beta$ tends towards unity, the shape function concentrates at forward directions. We found that the benchmark partial-wave shape functions of Kissel *et al.*[4] can be closely approximated by the analytical form, Eq. (5), if one sets $\beta' = \beta(1+B)$ and considers $A$ and $B$ as adjustable parameters. The parameters $A$ and $B$ have been determined, by least squares fitting, for the 144 combinations of atomic number, electron energy and reduced photon energy corresponding to the benchmark shape functions tabulated by Kissel *et al.*[4] Results of this fitting are compared with the original partial-wave shape functions in Fig. 1. The largest differences between the fits and the data were found for the higher atomic numbers, but even then the fits are very accurate. The quantities $\ln(AZ\beta)$ and $B\beta$ vary smoothly with $Z$, $\beta$ and $\kappa$ and can be obtained by cubic spline interpolation of their values for the benchmark cases. This permits the fast evaluation of the shape function for any combination of $Z$, $\beta$ and $\kappa$.

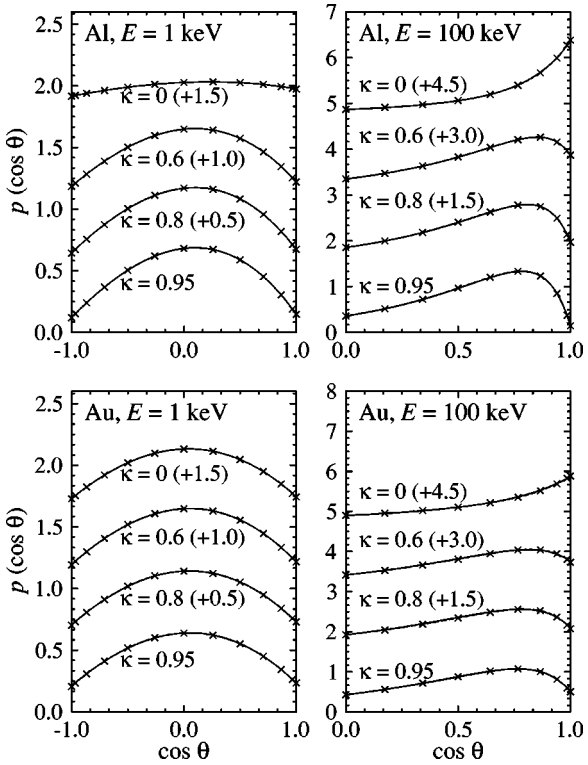


FIG. 1. Shape functions (angular distributions) for bremsstrahlung emission by electrons of the energies indicated in the fields of Al and Au atoms. The symbols indicate the partial-wave shape functions of Kissel *et al.* (Ref. 4). Continuous curves are the present analytical fits, Eq. (5). As a visual aid, some curves were shifted upward by the amounts indicated in parentheses.

Let us now consider the simulation of radiative events from the DCSs defined by Eqs. (1) and (5). The scaled DCS is interpolated from Seltzer and Berger's data,[3] in such a way as to allow accurate (and fast) linear interpolation in the variable $\ln E$. The random sampling of $\cos\theta$ is simplified by noting that the PDF given by Eq. (5) results from a Lorentz transformation, with speed $\beta'$, of the PDF, Eq. (3). This means that we can sample the photon direction $\cos\theta'$ in the reference frame K$'$ from the PDF, Eq. (3), and then apply the transformation, Eq. (4) (with $\beta'$ instead of $\beta$) to get the direction $\cos\theta$ with in the laboratory frame. To generate random values of $\cos\theta$ from Eq. (3) we use an algorithm which combines the composition and rejection methods (see Ref. 9 for details).

The bremsstrahlung simulation algorithm described above has been implemented into the Monte Carlo code system PENELOPE[9] (an acronym for penetration and energy loss of positrons and electrons), a general-purpose Monte Carlo subroutine package for the simulation of coupled electron–photon transport. The complete code system is available from the NEA Data Bank.[10] In what follows, results from simulations of thick-target bremsstrahlung with PENELOPE are compared with experimental data.

Figure 2 shows thick-target bremsstrahlung spectra produced by 70 keV electrons impinging 45° on the surface of a 50.7 mg/cm$^2$ thick slab of tungsten. Emission angles of 45° and 90° with respect to the incident beam in transmission configuration are considered. The experimental spectra were

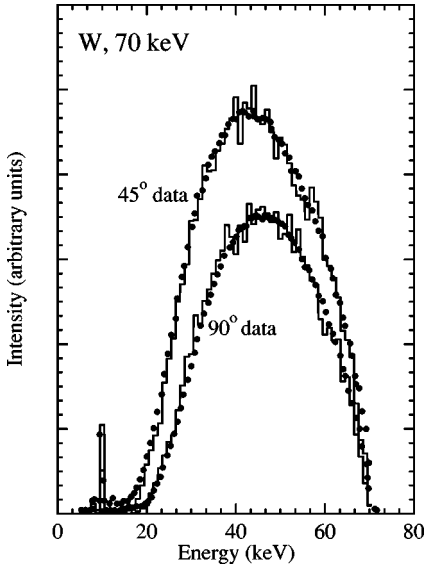


FIG. 2. Thick-target bremsstrahlung spectra produced by electrons impinging 45° on the surface of a 50.7 mg/cm$^2$ slab of tungsten. Spectra were collected at 45° and 90° with respect to the incident beam. Continuous curves are the results obtained from PENELOPE and symbols are data of Ambrose *et al.* (see Ref. 11).

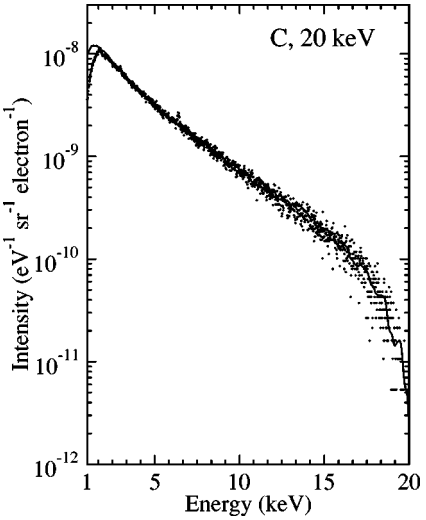


FIG. 3. Simulated (solid lines) and experimental (dots) x-ray spectrum, per incident electron, as a function of the photon energy radiated, generated by 20 keV electrons impinging normally on a thick slab of carbon; the detection angle is 130°.

measured by Ambrose *et al.*[11] For the present comparison, experimental spectra were scaled to the simulated ones by making the areas under the spectra equal, excluding the region of characteristic x rays. The simulation results are seen to be in excellent agreement with the experimental data.

In Fig. 3 we show simulated and experimental bremsstrahlung spectra produced by 20 keV electrons impinging normally on a thick slab of carbon. The experimental spectrum was obtained using a Cameca SX-50 electron microprobe, equipped with a Si(Li) detector. In this case, the emission angle is 130° with respect to the incident beam (i.e., reflection configuration). Notice that both the simulated and measured spectra are given in absolute units. In the present comparison, we have assumed an energy-dependent Gaussian energy-resolution profile. Because of the thicknesses of the Si(Li) crystal ($\sim$3 mm) and the berillium window (7 $\mu$m), comparison of simulated and measured spectra is meaningful for the photon energy range of $\sim E = 3-15$ keV, where the detector's efficiency can be assumed to be unity. The simulated spectrum is in excellent agreement with the experimental data in this photon energy range.

It can be concluded that the proposed algorithm provides a fast and accurate method for sampling the energy and direction of bremsstrahlung photons. The parameterization, Eq. (5), of the shape function gives a very accurate fit of Kissel *et al.*'s[4] benchmark data and, therefore, the simulated angular distributions are fully consistent with the most reliable theory. However, it is worth noting that calculated shape functions are available only for a quite sparse grid of energies $E$ and atomic numbers $Z$ and, consequently, interpolation in these variables may introduce appreciable uncertainty. To ensure the reliability of the algorithm in general-purpose Monte Carlo simulations, it is desirable to have calculated shape functions for a denser grid of energies and atomic numbers. Nevertheless, the results from the present simulations of thick-target bremsstrahlung spectra for carbon and tungsten, which do not belong to the set of benchmark cases, are found to be in good agreement with the experiments.

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