Numerical simulation of electron-impact x-ray sources

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ABSTRACT

Electron-impact x-ray sources will be used to calibrate the Advanced X-Ray Astrophysics Facility (*AXAF*), and models of the source x-ray spectra are necessary in forecasting the calibration performance.

We simulate the spectra of x-ray lines and continumm (0.1 - 13 keV) arising from electron impact on solid targets. We use simple models for electron transport, line and continuum emissivities, and radiative transport through the target. The electrons are attenuated in energy in the target but are unscattered in direction. The continuum x-ray emission is modeled as bremsstrahlung, and the characteristic x-ray line emission is modeled by electron collisional ionization followed by radiative decay to form the lines. X-ray attenuation is also included in the radiative transfer through the target. Multilayer or compound targets can be easily treated.

We compare the spectra produced by this model to the model of Pella *et al.*[2] and data from metal targets.[3]

Keywords: electron-impact x-ray sources, numerical modeling

1 INTRODUCTION

The Advanced X-ray Astrophysics Facility (*AXAF*) constitutes the x-ray component of NASA's "Great Observatories" program, and will provide high-resolution imaging and high-resolution dispersive spectroscopy of astrophysical x-ray sources.[1] A precision calibration of the *AXAF* telescope and science instruments will be performed by the *AXAF* Team, using x-ray sources located at NASA's X-Ray Calibration Facility (XRCF) at Marshall Space Flight Center.

Some of these x-ray sources will involve electron-impact on over twenty different targets spanning a range of atomic number $4 \leq Z \leq 79$, including some compounds. A tool to predict the spectra of x-rays from these sources is necessary for the *AXAF* calibration planning to predict the detected spectra and count rates that will be observed from the various combined telescope and detector calibrations. In this paper we discuss the development of a model (§2) to simulate both the line and continuum spectra for x-ray energies $0.1\,\mathrm{keV} \lesssim \mathrm{E} \lesssim 13\mathrm{keV}$ arising from electron impact on solid targets. We compare our model results (§3) with that of Pella *et al.*[2] and with data of x-ray spectra from a Manson source at MIT.[3]

2 TARGET MODEL

Although semi-empirical models exist to calculate the x-ray emission for electron-collision targets (*e.g.*, Pella[2]), we have used simple but *fundamental models* to represent the microphysics of electron transport and x-ray production within the target. This approach allows us to model the target without macroscopic parameters derived from previous measurements of electron-impact x-ray spectra (such as line–to–continuum ratios) that must be included in semi-empirical models. For example, Pella *et al.*[2] compiled parameters to determine only the $K\alpha$, $K\beta_1$, $L\alpha_{1,2}$ and $L\beta_1$ lines, using x-ray data from targets with $24 \leq Z \leq 74$. Determining the intensities of other lines requires additional data, and extrapolation of model parameters to atomic numbers outside of the Cr - W region may be problematic. In our approach, we specify the problem at a more fundamental level, using parameters that determine electron energy loss, ionization cross sections, x-ray radiative transition probablitites, and mass attenuation coefficients. Such an approach also makes simulating multilayer or compound targets a straightforward extension to simulating a monolithic target.

2.1 Electron Transport

The electrons are represented by a "uniform attenuated beam" model, hereafter referred to as "AB"; electrons of a given initial energy and current density are incident normal to the surface of the target, and are not deflected in direction during passage through it (*i.e.*, no backscattering). The electrons are uniformly attenuated in energy, with the energy loss given by the Bethe-Bloch formula.[6] No "energy straggling" is included in this calculation, so that there is one–to–one correspondence of electron energy and electron depth in the target. The energy I in the energy-loss formula that characterizes the binding of the electrons in the target is given by $I \simeq 16Z^{0.9}$ eV.[5] The energy loss of a compound target is approximated by $dE/dx \simeq \sum(dE/dx)_m$, where subscript m designates the energy-loss for the element m in the target, weighted by the appropriate fractional density.[6] The attenuation of the electrons is stopped when the electron energy $E \leq 20$ eV. Electron production caused by x-ray photoionization is not included.

2.2 X-Ray Continuum Emission

We calculate the continuum x-ray emissivity from a bremsstrahlung differential cross section using either the Bethe-Heitler[7] formula, or that from a screened-bremsstrahlung theory using a Thomas-Fermi model for the atom.[8] The cross section is taken to be isotropic in angle between the projectile electron and emitted photon. This cross section is combined with the target density, and local flux density of the electrons to determine the local volume emissivity of the target. Here again, it is straightforward to handle multilayer or compound targets. The results we present here use the Bethe-Heitler bremsstrahlung cross section.

2.3 X-Ray Line Emission

The catalog of Bearden[9] provides the energies of the characteristic lines of the target elements. The volume emissivity for the production of the spectral lines is calculated using the electron collisional ionization cross sections for the parent atomic (sub)shells, combined with the specific line transition probabilities and the local electron flux density. The ionization cross sections are those tabulated in the Livermore Evaluated Electron Data Library,[11] fit to a simple function of electron energy. The line transition probabilities are derived from the radiative rates of Scofield[13] and the nonradiative rates of Chen, Crasemann, and Mark,[14] or in the case of ionizations from shells $\geq$M from the Livermore Evaluated Atomic Data Library.[12] Some transition probabilities are also estimated from the radiative yields compiled by Krause.[16]

2.4 X-Ray Attenuation and Radiative Transfer

X-ray attenuation is included as part of the radiative transfer of x-rays within the target. The element mass absorption coefficient (including incoherent scattering) is that of a polynomial in powers of E^{-1} derived by Biggs and Lighthill.[17] The equation of radiative transfer[15] is then solved at specific photon energies through the target for a numerical accuracy of a few percent.

3 COMPARISONS OF AB MODEL TO PELLA MODEL AND DATA

Figures 1a,b show the continuum spectrum produced by the AB model compared to that produced by the Pella model, for a Cu target at 5 and 30 kV. The takeoff angle for both of these simulations is taken to be 45°. There is agreement within a factor of ~ 2 between the Pella and AB model over a wide range of photon energies, with larger discrepancies for lower ($\lesssim 0.1$ keV) energies and also toward the target cutoff energy. Figure 2 shows a comparison of $K\alpha$ and $K\beta$ line intensities, as a function of target voltage. The AB model produces smaller line yields at lower target voltages. However, the Pella model may also produce insufficient line intensity for lower Z targets (see below).

Figures 3a-d show the comparison of the AB model for Mo, Ti, Cu, and MgO targets with data taken with a Manson Model 5 multi-anode source (takeoff angle of 45°).[3,4] A solid state detector ($\Delta E \simeq 140$ eV FWHM) was used to collect the data, and the detector's resolution and efficiency have been included in the model spectra.

The plots show agreement of the model and data within a factor of 2–3 over a wide range of energies, with larger disagreement at photon energies near the cutoff energy and below $\simeq 0.7$ keV. Both the model continuum and line intensities appear to be lower than the data by similar factors, and all four target models are all lower than the data by similar factors. Note that only the model for the MgO target has more than one element (Mg and O) been included; no attempt has been made to incorporate the contaminants seen in the spectra (C, O, Si, W, etc.). Also included in these plots are simple fits of the data using the Kramer's formula[10] for the observed continuum, and line intensities calculated from Pella. No attenuation effects by the target have been included. In many cases (*i.e.*, lower-Z elements) the Pella-estimated line intensities were substantially smaller than that observed.[3] Therefore, the Pella-estimated line intensities for the have been arbitrarily adjusted to provide a good fit to the data.

Figure 1: The x-ray continuum spectrum produced by the Pella model (solid squares) and the AB model (open triangles) for a Cu target at (a) 5 kV and (b) 30 kV. The takeoff angle for both simulations is 45°.

4 CONCLUSIONS

We have simulated the spectra of x-ray lines and continumm arising from electron impact on solid targets, using simple model to describe electron transport, x-ray line and continuum emissivities, and radiative transport through the target. We have found that this relatively simple model can produce surprisingly good fidelity (within factors of $\sim 2-3$) with the models of Pella *et al.*[2] and and with observed x-ray spectra from electron-impact sources. Work is currently underway to include additional physics (*e.g.*, more realistic electron transport via a Boltzmann-equation description and nonisotropic bremsstrahlung) to provide reliable tool to predict x-ray source spectra.

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Figure 2: The $K\alpha$ and $K\beta$ line intensities produced by the Pella (solid symbols) and AB (open symbols) models for a Cu target, as a function of target voltage.

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Figure 3: The x-ray spectra measured from a Manson source for (a) Mo, (b) Ti, (c) Cu, and (d) MgO targets, compared with the AB model simulations. Detector effects are included. Also shown (solid line) are best fits provided by a simple Kramers model for the continuum; line emission has been also included, but the line intensities have been arbitrarily adjusted to improve the fit to the data.

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