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MC X-Ray, a New Monte Carlo Program for Quantitative X-Ray Microanalysis of Real Materials

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This paper will present a new Monte Carlo program, MC X-Ray. This new program is an extension of the Monte Carlo programs Casino [1] and Win X-Ray [2] since it computes the complete x-ray spectra from the simulation of electron scattering in solids of various types of geometries. This new program, which has been completely reprogrammed in C++ under a window environment, is a real improvement because Win X-Ray is only able to compute x-ray spectra of homogeneous materials and CASINO performs only the computation of net x-ray intensities in a limited set of geometries. MC X-Ray allows more than 100 different regions in the materials having shape of spheres, cylinders and combinations of horizontal and vertical planes. All these regions can have a different composition.

MC X-Ray includes the Bremstrallung cross-sections of Ding – Statham to compute the emitted background x-ray intensity. Figure [1] shows a comparison between the Kirkpatrick – Wiedmann, used in Win X-Ray, and the Ding – Statham cross sections for Au at 20 keV. The Ding – Statham cross sections results in a spectrum that is flatter, a critic often made about spectra simulated by Win X-Ray. Figure [2] shows a true EDS spectrum detected by a Si(Li) detector computed from the simulation of the absorption of 50 000 photons and the diffusion of the photo-electrons in the EDS detector using the spectra of figure [1]. MC X-Ray simulates the true noise of EDS spectra without using Gaussian noise techniques. Figure [3] and [4] show simulated C and Cu K_α maps of a 40 nm carbon nanotube filled with a 10 nm cylinder of Cu at 20 keV and with a probe diameter of 1 nm. Clearly, MC X-Ray is a useful tool for x-ray microanalysis since it has many more features.

References

1. P. Hovington, D. Drouin and R. Gauvin (1997), “Casino: A New Era of Monte Carlo Code in C Language for Electron Beam Interaction, Part I: Description of the Program”, Scanning, Vol.19, pp. 1-14.
2. R. Gauvin, E. Lifshin, H. Demers, P. Horny and H. Campbell (2003), “Win X-ray, a new Monte Carlo Program that Computes X-ray Spectrum for X-ray Microanalysis in the Scanning Electron Microscope”, Submitted to Microscopy & Microanalysis.

Figure [1] Simulated x-ray spectra of Au at 20 keV with 2 models of Bremstrallung cross-sections.

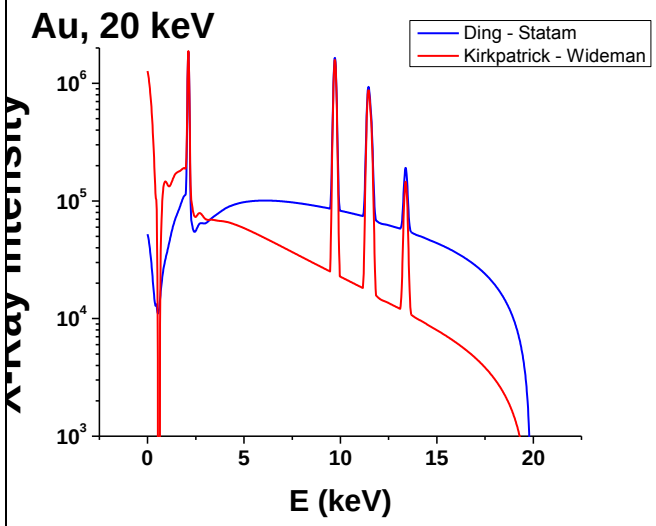


Figure [2] Simulated EDS spectra of a Si (Li) detectors with the absorption of photons in the detector and the subsequent scattering of the photo-electron.

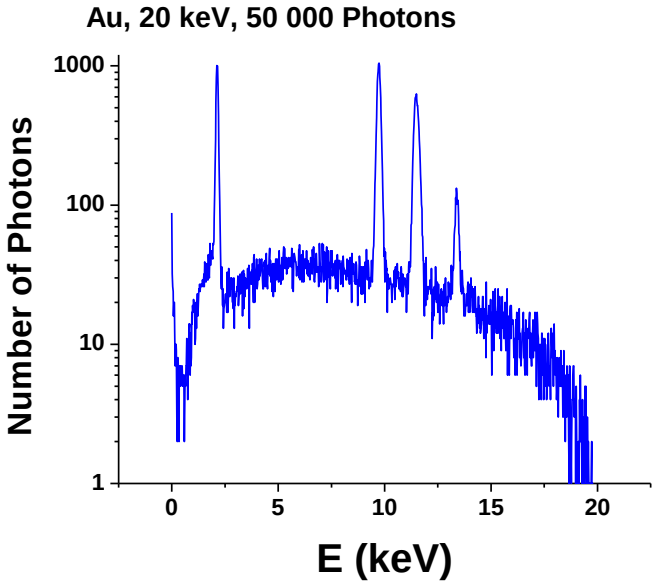


Figure [3] Simulated C K_α map of a 40 nm carbon nanotube filled with a 10 nm cylinder of Cu. 20 keV and D = 1 nm.

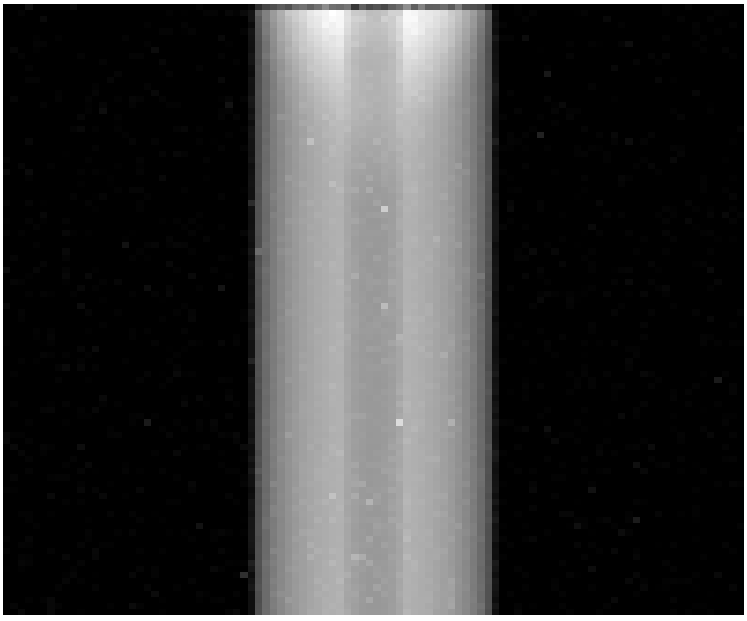
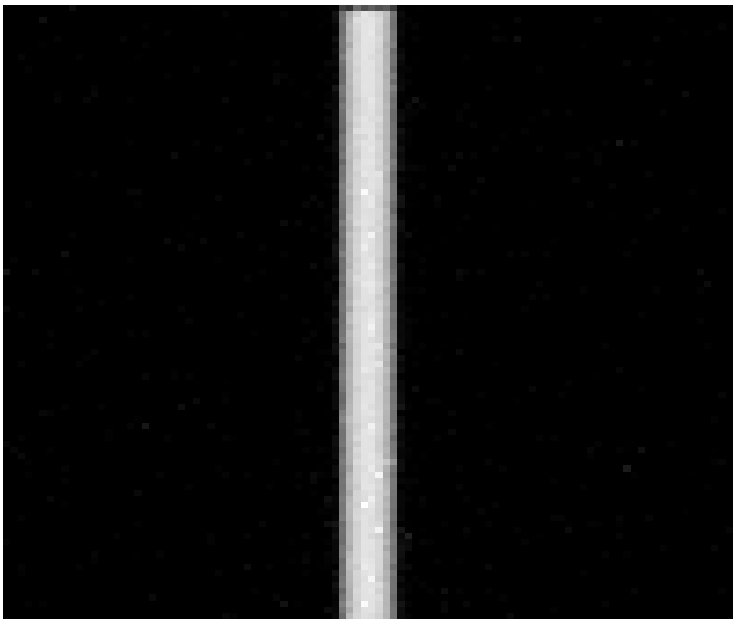


Figure [4] Simulated Cu K_α map of a 40 nm carbon nanotube filled with a 10 nm cylinder of Cu. 20 keV and D = 1 nm.



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