Quantitative X-Ray Microanalysis of Real Materials in Electron Microscopy with Monte Carlo Simulations.

Raynald Gauvin<sup>1</sup>, Pierre Michaud<sup>1</sup> and Michel L. Trudeau<sup>2</sup>

<sup>1</sup>Department of Materials Engineering, McGill University, M. H. Wong Bldg, 3610 University Street, Montreal, Québec, Canada, <sup>2</sup> Chimie et MatériauxScience des Matériaux, Centre Institut de Recherche d'Hydro-Québec, 1800 Boul. Lionel-Boulet, Varennes, Québec, Canada

Electron microscopy has two main emerging areas of applications, low voltage field emission scanning electron microscopy (FE-SEM) and high voltage field emission transmission electron microscopy (FE-TEM) with spherical aberration correctors. In the first case, the reduction of the electron beam energy leads to improved spatial resolution for x-ray microanalysis but when the beam energy is too low, the vield of generated x-rays becomes too small. In the second case, a probe diameter of the order of 1 Å with high current can be obtained with a spherical aberration corrector. Coupled with the high energy of the electron beam that penetrates almost in a straight line through the transparent material, high spatial resolution can be achieved. However, beam damage and specimen preparation issues are still of concerns. Focus Ion Beam (FIB) has helped in fixing problems related to specimen preparation for FE-TEM. But, since the FIB allows making thin films of different materials, imaging in FE-SEM in the STEM mode is now possible, as well as x-ray microanalysis in these conditions. Therefore, we now have to see x-ray microanalysis as a characterization technique that can be used between 3 to 300 keV of electron beam energy on complex materials having various shapes and phases and or regions of different composition. This paper presents applications of MC X-Ray, a new Monte Carlo program that allows simulating x-ray spectra in materials of various phases of different composition and size with electron beam energy between 1 to 400 keV. Results for quantitative x-ray microanalysis obtained in a FE-SEM (Hitachi SU-8000) at low beam energy and in a FE-STEM (Hitachi HD-2700 with Cs corrector) at 200 keV will be presented. As an example of the capabilities of MC X-Ray, Figure [1] shows a 400 X 400 CKα map simulated for a 1 µm W sphere on top of bulk C at 20 keV with 50 e/pixel with a TOA of 40°. The absorption of the C K $\alpha$  in the W sphere is clearly visible. Since the variation of C K $\alpha$  intensity is due to absorption variation, not composition variation, correct modeling of x-ray absorption with Monte Carlo simulations is required for accurate quantitative x-ray microanalysis. Figure [2] shows the peak to background ratio of the C Kα line and the Pd and Sn lines for a 2 nm Pd – Sn spherical particulate on top of a 10 nm carbon nanotube as a function of beam energy. Optimum beam energies can be predicted.

