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Calculated X-ray Intensities Using Monte Carlo Algorithms: A Comparison To Experimental EPMA Data

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Monte Carlo (MC) modeling has been used extensively to simulate electron scattering and x-ray emission from complex geometries. Here are presented comparisons between MC results and experimental electron-probe microanalysis (EPMA) measurements as well as $\phi(\rho z)$ correction algorithms. Experimental EPMA measurements made on NIST SRM 481 (AgAu) and 482 (CuAu) alloys, at a range of accelerating potential and instrument take-off angles, represent a formal microanalysis data set that has been widely used to develop $\phi(\rho z)$ correction algorithms. X-ray intensity data produced by MC simulations represents an independent test of both experimental and $\phi(\rho z)$ correction algorithms. The α-factor method has previously been used to evaluate systematic errors in the analysis of semiconductor and silicate minerals, and is used here to compare the accuracy of experimental and MC-calculated x-ray data [1-3]. X-ray intensities calculated by MC are used to generate α-factors using the certificated compositions in the CuAu binary relative to pure Cu and Au standards. MC simulations are obtained using the NIST, WinCasino, and WinXray algorithms; derived x-ray intensities have a "built-in" atomic number correction, and are further corrected for absorption and characteristic fluorescence using the PAP $\phi(\rho z)$ correction algorithm [4-7]. The Penelope code additionally simulates both characteristic and continuum x-ray fluorescence and thus requires no further correction for use in calculating α-factors [8].

Preliminary results for α-factor analysis of Cu Kα and Au Lα in SRM 482 at 20 kV and 40 degree takeoff angle are shown in figures 1 and 2. For these data there is ~ 5-10% agreement between intensities calculated by MC and the PAP $\phi(\rho z)$ algorithm compared to experimental EPMA data acquired on three different electron microprobes at NIST, Caltech, and Marshall Space Flight Center. The range for replicate EPMA measurements (Caltech $Cu_{80}Au_{20}$) compares favorably with measurement range for the three laboratories, and is also comparable to the range of results for MC and $\phi(\rho z)$ algorithms. The WinXray and Penelope packages produce an energy spectrum that permits comparison with experimental EDS spectra, and can be used to perform detector modeling. The Penelope results presented here were obtained using a modified version of the code which is optimized for calculation of characteristic x-ray intensities. The good agreement indicates that MC modeling can be successfully used to calculate x-ray intensities for quantitative EPMA. Results of application to silicate minerals, thin films, and other examples will be presented.

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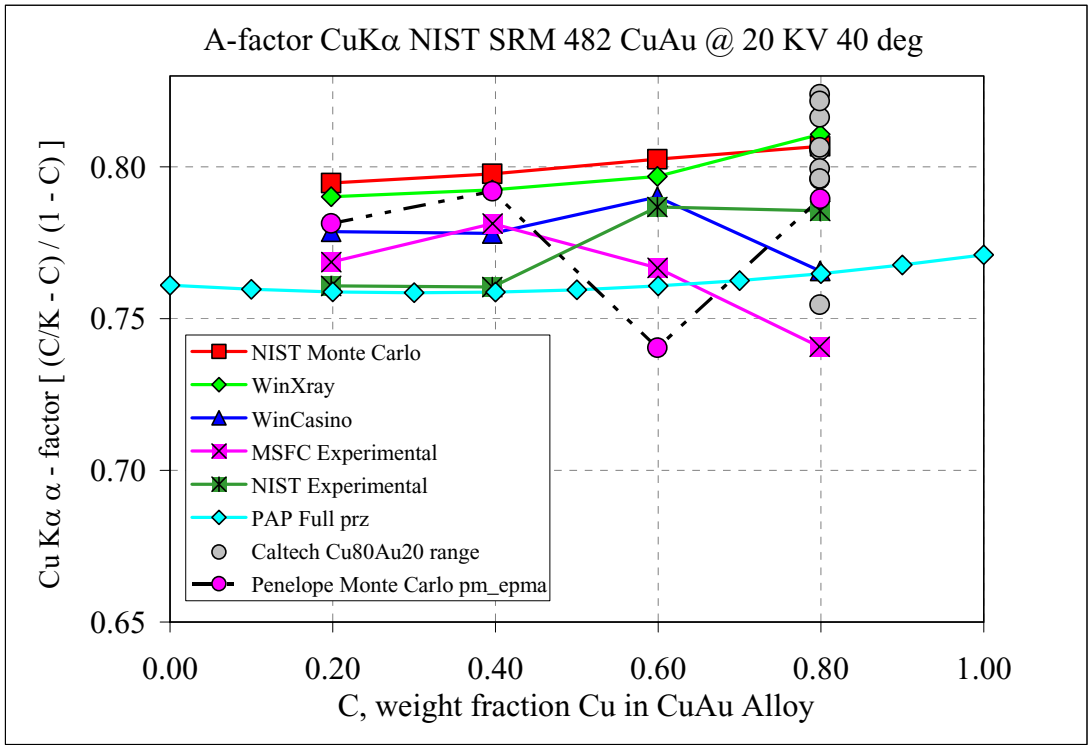

Figure 1 Cu Kα α-factors in CuAu binary using NIST SRM 482 CuAu compositions. Calculated data values using NIST, WinXray, WinCasino, and Penelope Monte Carlo algorithms, compared with PAP full ϕ(ρz) calculated values, and experimental EPMA data from NIST, Caltech, and Marshall microprobes. Range of typical replicate measurements indicated for Caltech $Cu_{80}Au_{20}$ alloy; compare with range for EPMA measurements.

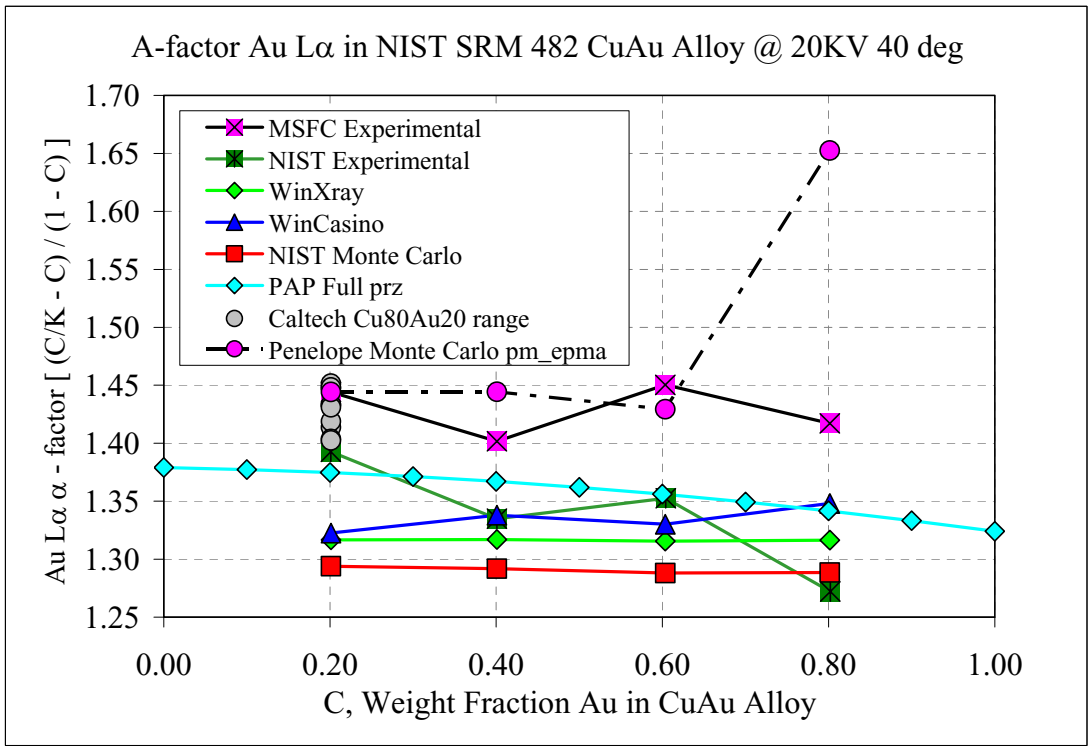

Figure 2 Au Lα α-factors in CuAu binary using NIST SRM 482 CuAu compositions.

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