ACCURACY OF FUNDAMENTAL PARAMETERS CALCULATIONS USING A NEW ATOMIC DATABASE

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A series of calculations and corresponding measurements were made to evaluate the accuracy of the fundamental parameters method using a new atomic database. The database is a recent compilation by Elam, Ravel, and Sieber [1] which is intended for x-ray spectroscopy. The measured XRF spectra from a number of standard specimens were analyzed by the fundamental parameters method without reference to any other standard. The predicted intensities were calculated using the primary and secondary fluorescence equations, accounting for Coster-Kronig transitions and fluorescence cascade effects. Incident spectra were calculated using the prescription of Ebel [2] but with atomic parameters from the new database.

The measurements were performed on an EDAX Eagle II spectrometer with a Rh tube operated under various conditions. The detector was a liquid-nitrogen-cooled Si(Li) crystal. The net peak intensities from the measured spectra were analyzed using the "pure" fundamental parameters method and the results compared to the certified values. Agreement was generally better than 1% absolute for a series of alloy and oxide samples. Complete results and statistical summaries will be presented. Trends in the errors were examined to ascertain the effects of neglecting tertiary fluorescence as well as bias in the atomic parameters.

[1] W.T.Elam, B.D.Ravel, and J.R.Sieber, *Radiation Physics and Chemistry* **63** (2002) 121–128.
[2] Horst Ebel, *X-ray Spectrometry* **28** (1999) 255-266.

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