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New measurements and calculations of inner-shell ionization cross sections by electron impact

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Accurate cross sections for inner-shell ionization by electron impact are needed for quantitative analysis by Auger electron spectroscopy (AES), electron energy-loss spectroscopy (EELS), analytical electron microscopy (AEM), and electron probe microanalysis (EPMA). In spite of this need, a systematic method to calculate ionization cross sections from first principles remains to be found. Cross sections calculated within the plane-wave Born approximation (PWBA) are reliable for high-energy electrons, but their accuracy deteriorates when the energy of the electron approaches the ionization threshold, because of the increasing distorting effect of the atomic field on the wave functions of the incident and emerging electron and the exchange effects. A more rigorous approach is provided by the distorted-wave Born approximation (DWBA) [1], in which the initial and final projectile wave functions include the distortion caused by the atomic field, allowing also the description of exchange effects. However, DWBA calculations are extremely time consuming and feasible only for a limited range of incident electron energies. Alternatively, a number of empirical and semi-empirical approximate formulas have been proposed [2]; among the most popular are the formulas of Casnati et al. [3] and Gryzinski [4]. The simplicity of these formulas makes them suitable for quantitative algorithms but unfortunately they have limited ranges of validity and accuracy. Indeed, most of the predictive formulas have been derived to reproduce experimental data, but these are scarce and affected by considerable uncertainties.

Measurements of inner-shell ionization cross sections for different elements and atomic shells have been performed by our group during the last years [5,6,7,8]. Specifically, the cross sections have been deduced from the x-ray intensity emitted by self-supporting ultra-thin films of the studied elements, which have been measured on the electron microprobe using both energy-dispersive and wavelength-dispersive spectrometry. A significant result from these studies is the good agreement between our measured data with the DWBA calculations, especially for the K-shell of medium-Z elements and the L-shells of high-Z elements. However, questions remain about the validity of the DWBA for the L-shells of medium and low-Z elements, for which the experimental data are very scarce and the DWBA calculations are limited to energies up to 10 times the ionization threshold. In this context, we have developed a new numerical algorithm that allows the calculation of cross sections within the DWBA for energies far above the ionization threshold [9]. In this communication, we describe in detail the experimental technique used in our measurements of inner-shell ionization cross sections and we report new measurements of the K-shell ionization cross section and the $L\alpha$ and $L\beta_1$ x-ray production cross section for several medium-Z elements by impact of electrons with energies from 1.5 keV up to 39 keV. For the K-shell of these elements, our results confirm the excellent agreement between the predictions of the DWBA with the experimental measurements. Conversely, the formulas of Casnati and Gryzinski are found to overestimate ($\sim$ 10%) and underestimate ($\sim$ 20%) our measurements, respectively. The situation is different for the *L*-shells: here the formulas of Gryzinski and Casnati seem to reproduce much better our measurements than the DWBA calculations, which overestimate the experimental data about 10-15%. Nevertheless, it should be noted that the uncertainties of the fluorescence yields and Coster-Kronig coefficients adopted in the calculations, which may amount up to 30%, make it difficult to draw a definite conclusion about the reliability of calculated cross sections for the *L*-shells of such elements.

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