Nuclear Instruments and Methods in Physics Research B 268 (2010) 1802–1805

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Simulation of L X-ray yields induced by He ions

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ARTICLE INFO

Article history:
Available online 25 February 2010

Keywords:
PIXE
X-rays
Simulation
Alpha particles

ABSTRACT

The PIXE simulation open-source library, LibCPIXE [1], publicly released, allows the simulation of X-ray yields of PIXE spectra taken from arbitrary samples irradiated with proton beams, including multilayered targets. Nevertheless, IBA analysis of many systems of interest to material sciences and other applications frequently require the quantification of He ions induced X-ray yields. LibCPIXE was thus adapted to this requirement. In this work, simulated intensities of the L lines are compared to the experimental results from W compound samples irradiated with He^{2+} ion beams [2]. Problems overcome or faced during this extension to He beams, including fundamental parameters details on the database and approximations used, are discussed.

1. Introduction

The quantitative characterisation of samples using several ion beams is fundamental in the study of new materials and new applications in material sciences, in particular using H^+ and He^{2+} ion beams. PIXE is an excellent IBA technique for this quantitative analysis.

The simulation of X-ray yields of multilayered samples is possible using LibCPIXE [1], which allows the simulation of X-ray yields of fully customised multilayered samples induced by proton beams. The first version of LibCPIXE, released in 2006, is able to simulate X-ray yields from a given arbitrary sample irradiated with H^+ beams and under general experimental conditions. LibCPIXE needs to be adapted to allow the simulation of X-ray yields induced by He^{2+} ion beams, becoming more versatile.

The LibCPIXE simulation code is based on the ECPSSR theory for X-ray production cross-sections and several corrections and approximations to X-ray production and ionisation cross-sections. Adapting LibCPIXE to the use ion beams other than protons requires a careful look at the calculation of the X-ray production cross-sections.

2. Simulation model considerations

As mentioned before, LibCPIXE was first developed to calculate the characteristic X-ray emissions produced by irradiation of a sample, including multilayered samples, with proton beams [1].

The number of characteristic X-rays, N_{ij} emitted by an element, i, due to an electronic transition, j, can be expressed for a layered sample as [1]

$$N_{ij} = \frac{\Omega}{4\pi}\epsilon_j N \sum_l \left[T_{jl} C_{il} \int_{E_{l,out}}^{E_{l,in}} \frac{\tau_{lj}(x(E))}{S_l(E)} \sigma_{ij}(E) dE \right] \quad (1)$$

where the l index accounts for each layer of the sample, $\Omega/4\pi$ is the detection solid angle fraction, ϵ_j is the detector efficiency for the energy of the j emission, N is the number of beam particles, C_{il} is the concentration of the element i in the l layer, T_{jl} is the transmittance for the j X-ray energy due to absorbers located between the surface of the layer l and the active area of the detector, $\tau_{lj}(x)$ is the transmittance between the position x inside the l layer and its surface, S_l is the stopping power for the beam particles in the layer l and σ_{ij} is the X-ray production cross-section for the impact of particles of energy E. $E_{l,in}$ and $E_{l,out}$ are the energies of the beam ions when entering and exiting the layer l, respectively.

Each line $X_{j,s}$ corresponding to an electron transition j to subshell s, has an associated X-ray production cross-section that can be written as

$$\sigma^X_{j,s} = k_{j,s}\omega_s V_s \quad (2)$$

where V_s is the final vacancy distributions defined by Bambynek et al. [3] as

$$\begin{aligned} V_3 &= (f_{12}f_{23} + f_{13})\sigma_1 + f_{23}\sigma_2 + \sigma_3 \\ V_2 &= f_{12}\sigma_1 + \sigma_2 \\ V_1 &= \sigma_1 \end{aligned} \quad (3)$$

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doi:10.1016/j.nimb.2010.02.078

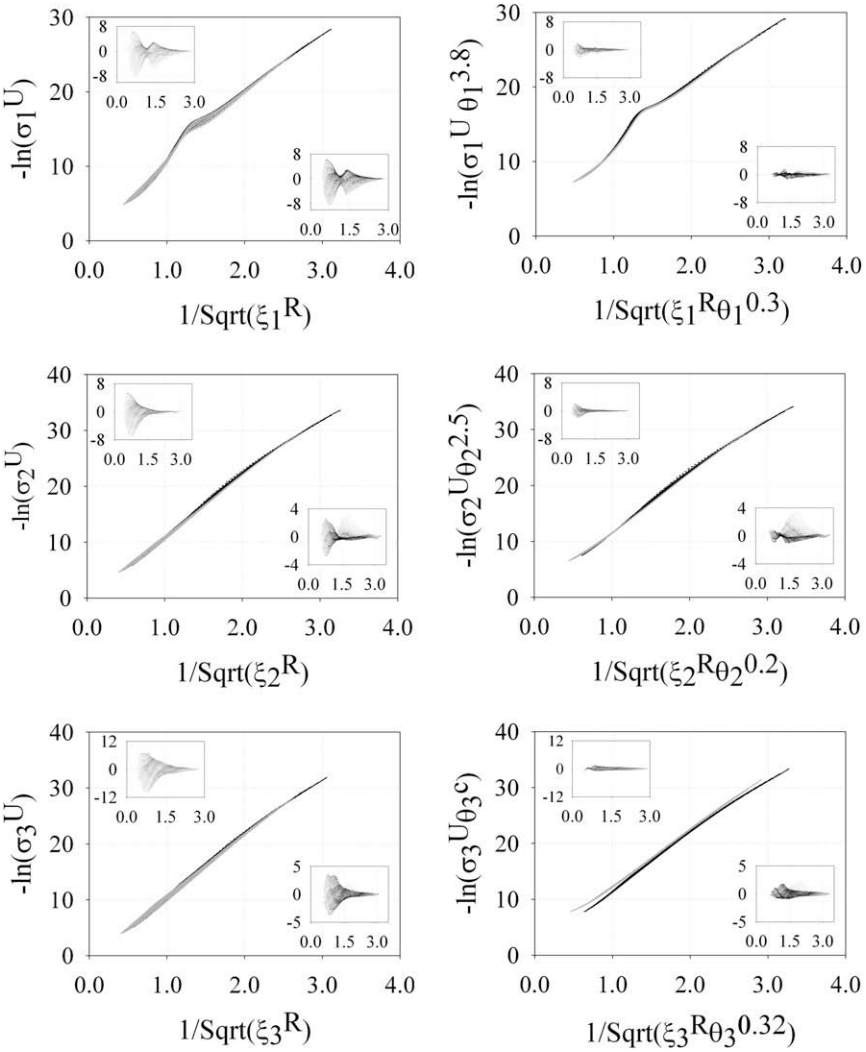

Fig. 1. Left hand side: universal ionisation cross-section displayed versus the reduced ion velocity for 60 elements, from $Z = 32$ to $Z = 92$, for H^+ (grey dots) and He^{2+} (black dots) ions, and for 70 energy values in the range of 50 keV to 9.5 MeV, in the H^+ case, and in the range of 100 keV to 10.0 MeV, in the He^{2+} ions case. Right hand side: rescaled universal ionisation cross-section displayed versus the rescaled reduced ion velocity for the several elements and energies for (grey dots) and He^{2+} (black dots) ions. Relative residuals of the polynomial fittings are presented in the top left corner of each graph for the H^+ case and in the bottom right corner, for the He^{2+} ions case.

f_{mn} being the Coster–Kronig coefficients, ω_s the fluorescence yields, $k_{j,s}$ the relative emission rates and σ_s the ionisation cross-section for each of the L sub-shells.

In the released version of the LibCPIXE code, the L X-ray production cross-sections for protons are calculated using a semi-empirical correction from Reis and Jesus [4], in combination with Coster–Kronig coefficients and fluorescence yields [5], the Scofield L lines relative emission rates [6] and an universal polynomial approximation to ECPSSR ionisation cross-sections [7] first established by Reis in 1993 but was unpublished in the standard literature. The semi-empirical correction to the X-ray production cross-sections by Reis and Jesus [4] is optimized for proton beams, so it was not applied in the calculation of the X-ray production cross-sections for He^{2+} ions. Furthermore, the use of Coster–Kronig coefficients and fluorescence yields values from Krause [5] instead of more recent recommended values from Campbell [8,9] also does not affect significantly the results obtained since slight differences originating from the use of different databases in this case are eroded on the experimental calibration process of the PIXE system yield.

Following the earlier work of Reis [7], the ECPSSR ionisation cross-sections can be expressed as

$$\sigma_s^{ECPSSR}(\xi_s^R, \zeta_s, \theta_s) = \frac{8\pi a_0^2}{\eta_s \theta_s}\left(\frac{Z_{proj}}{Z_s}\right)^2 C_s(x)\sigma_s^U \tag{4}$$

where ξ_s^R is the relativistic reduced ion velocity, ζ_s is the binding correction, θ_s is the reduced binding energy, η_s is the reduced incident ion energy, a_0 is the Bohr radius, Z_{proj} is the projectile atomic number and $Z_s = Z_{target} - 4.15$ is the target effective atomic number in Slater's shielding approximation for the L shell [3], using the same notation as Brandt and Lapicki [10,11], $C_s(x)$ is the Coulomb deflection correction defined by Brandt and Lapicki [10–12] and σ_s^U is the universal ionisation cross-section, which may be written as

$$\sigma_s^U = \frac{\sigma_s^{ECPSSR}(\xi_s^R, \zeta_s, \theta_s)}{8\pi a_0^2\left(\frac{Z_{proj}}{Z_s}\right)^2 C_s(x)}\eta_s\theta_s \tag{5}$$

Using an adapted version of the computer code used by Reis to calculate the 1996 tables [4], σ_s^U was evaluated by integrating the form factors over the exact range of momentum and energy transfer Q and W, for 60 elements with atomic numbers from $Z_{target} = 32$ to $Z_{target} = 92$, considering proton, $Z_{proj} = 1$, and He^{2+} ion, $Z_{proj} = 2$,