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Technical note

Disparity in formulations used for fluorescent X-ray intensity measurements

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ABSTRACT

The paper presents a problem in computations of X-ray fluorescence cross-sections, shell/sub-shell fluorescence yields, Coster–Kronig yields, vacancy alignment, etc. from X-ray fluorescence (XRF) studies. While using barn/atom as a unit for cross-sections if the atomic masses are not considered it causes a discrepancy in the measured cross-section, yield and alignment values. Most of the earlier publications are being quoted where such an oversight has occurred and discrepancy is evident.

1. Introduction

The process of inner shell vacancy creation by photon bombardment of target atoms and resulting in emission of characteristic X-rays on the decay of vacancies is called X-ray fluorescence (XRF). Accurate measurements of fluorescent X-ray intensities are required for the solution of many practical problems, e.g. the standardization of radioisotopes, design of many radiation detection devices, radiation transport in materials, atomic structure studies and to check theory against experiment. Analytical methods based upon X-ray fluorescence radiation have found wide applications in medical research, trace element analysis, non-destructive testing, etc. Since, the early eighties of twentieth century, various groups all over the world are engaged in XRF studies with fluorescent X-ray intensity measurements using direct sources of photons (X-rays, gamma rays and synchrotron photons) or external conversion X-rays in a variety of experimental setups using different types of photon spectrometers.

On examination of most of the published experimental work on fluorescent X-ray intensity measurements for X-ray fluorescence cross-sections (Kumar et al., 1982, 1985, 2001; Garg et al., 1985, 1986; Singh et al., 1987; Mann et al., 1990a, 1990b, 1991; Rao et al., 1993a, 1993b, 1994, 1995, 1996; Allawadhi et al., 1995; Puri et al., 1996, 1999; Budak et al., 1999; Barrea and Bonzi, 2000, 2001; Simsek, 2000a; Durak and Ozdemir, 2001; Ertugrul, 2001a, 2001b, 2002a; Kaya et al., 2001; Mandal et al., 2001; Tirasoglu et al., 2001; Bastug et al., 2002; Singh et al., 2003; Apaydin et al., 2005, 2008; Sharma et al., 2006; Han et al., 2007, 2010; Ozdemir, 2007; Chauhan et al., 2008; Küçükönder et al., 2008; Gupta et al., 2010a), shell/sub-shell fluorescence yields (Rao et al., 1995, 1996; Simsek, 2001; Kaya et al., 2001; Singh et al., 2003; Seven, 2004; Apaydin et al., 2005; Puri and Singh, 2006; Han et al., 2007; Chauhan et al., 2008; Tirasoglu and Sogut, 2008), Coster–Kronig yields (Simsek, 2000b, 2001; Oz et al., 2001; Ertugrul, 2002a, 2002b; Singh et al., 2002; Sogut et al., 2002; Puri and Singh, 2006; Cengiz et al., 2008; Chauhan et al., 2008; Gupta et al., 2010b), vacancy alignment (Kahlon et al., 1990, 1991a, 1991b; Ertugrul et al., 1995, 1996; Sharma and Allawadhi, 1999; Mehta et al., 1999; Demir et al., 2000; Kumar et al., 2001; Seven and Kocak; 2001, 2002; Seven, 2004; Barrea et al., 2005; Ozdemir et al., 2005; Sharma et al., 2006; Kumar et al., 2008; Ozdemir and Durak, 2008), etc. a disparity in the basic formulation has been noticed. The formulation expresses the emitted X-ray counts in terms of exciting photon source strength, experimental setup parameters, number of atoms/g of target material, detector efficiency and the probability of X-ray emission (fluorescence cross-section) being elaborated in the following text.

2. Basic formulation for measurements of fluorescent X-ray intensities

When a target is irradiated with photons from source and the resulting X-rays are counted in a detector (Fig. 1), the X-ray counts N_X under the photo peak in terms of basic parameters and the experimental setup parameters are given as

$$N_X = S_0 \frac{\Omega_1}{4\pi}\frac{\Omega_2}{4\pi} a_{air}(i) a_{air}(e) \varepsilon(e) \frac{A}{M} t \sigma^*(cm^2) \beta(i,e) \tag{1}$$

The terms source strength S_0, solid angles of target with source and with detector $\Omega_1/4\pi$ and $\Omega_2/4\pi$ respectively, air absorption corrections $a_{air}(i)$ and $a_{air}(e)$ at incident (i) and emitted (e) photon

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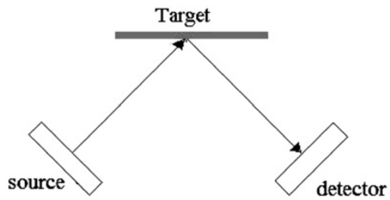

Fig. 1. Arrangement of source, target and detector.

energies and detector efficiency $\varepsilon(e)$ at emitted X-ray energy are dimensionless experimental setup parameters.

The target factor (A (Avogadro's number)/M(M.wt.))t(g/cm^2) is the target atoms/unit area with dimensions cm^{-2}.

The factor $\beta(i,e)$ is a dimensionless self-absorption correction factor for target material at incident (i) and emitted (e) photon energies.

σ^* is a fundamental parameter that represents the probability of X-ray emission and is expressed as $\sigma^* = \sigma_I \omega$, where σ_I is the ionization cross-section of the atomic shell and ω is its fluorescence yield.

To make right hand side dimensionless, σ_I values must be in barn (cm^2).

Moreover, the factor $\sigma_I(A/M)$ expresses σ_I in cm^2/g (Hubbel, 2006) i.e. σ^* is in cm^2/g. (the conversion factor from barn to cm^2/g is $(A/M)10^{-24}$). The relation (1) with σ^* in cm^2/g reduces to the form

$$N_X = S_0 \frac{\Omega_1}{4\pi}\frac{\Omega_2}{4\pi} a_{air}(i) a_{air}(e) \varepsilon(e) t \sigma^*(\mathrm{cm}^2/\mathrm{g}) \beta(i,e) \quad (2)$$

Generally, in the X-ray measurements the factor $I_0 G = S_0(\Omega_1/4\pi)(\Omega_2/4\pi) a_{air}(i)$ is the intensity of exciting radiation falling on the area of target that is visible to the detector. Therefore, the formulation used in the calculation of XRF cross-section is either

$$\sigma^*(\mathrm{barn}) = \frac{N_X M}{I_0 G A \beta(i,e) a_{air}(e) \varepsilon(e) t} \quad (3)$$

or

$$\sigma^*(\mathrm{cm}^2/\mathrm{g}) = \frac{N_X}{I_0 G \beta(i,e) a_{air}(e) \varepsilon(e) t} \quad (4)$$

In most of the latter measurements, the formulation relation (4) has been used but the cross-section values reported are in barn or no dimensions of cross-sections are mentioned. This raises the doubt about authenticity of data values quoted in the publications.

Moreover, for L/M X-ray measurements, detector efficiency and air absorption of emitted X-rays along with incident flux factor ($I_0 G a_{air}(e)\varepsilon(e)$) are determined in a separate experiment in the same setup. For this purpose the targets whose K X-rays energies are in the range of L/M X-ray energies of actual target and of the same dimensions as that of the target are irradiated with the same incident flux of photons and the emitted K X-rays are counted in the detector as N_{Kx} and the factor is given as

$$I_0 G a_{air}(e) \varepsilon(e) = \frac{N_{Kx} M_K}{\sigma_K^*(\mathrm{barn}) \beta_K(i,e) t_K A} \quad (5)$$

or

$$I_0 G a_{\mathrm{air}}(e) \varepsilon(e) = \frac{N_{Kx}}{\sigma_K^*(\mathrm{cm}^2/\mathrm{g}) \beta_K(i,e) t_K} \quad (6)$$

where all the terms have same meaning as in relation (1) except that they correspond to K X-rays instead of L/M X-rays.

3. Discussion on formulation used in computation of XRF cross-sections

Most of the published result evaluations are found with pair of relations (4) and (6). However, depending upon the dimensions of used σ_K^* values (barn or cm^2/g), the following possibilities of calculated values of $\sigma_{L/M}^*$ arise;

1. The use of σ_K^* values and evaluated $\sigma_{L/M}^*$ in cm^2/g are correct.
2. With the use of σ_K^* values in barn in relation (6) and evaluated $\sigma_{L/M}^*$ in barn from relation (4) (Garg et al., 1986; Rao et al., 1993a, 1993b, 1994; Puri et al., 1996; Budak et al., 1999; Simsek, 2000a; Barrea and Bonzi, 2000, 2001; Ertugrul, 2001a, 2001b, 2002a; Mandal et al., 2001; Singh et al., 2003; Sharma et al., 2006; Han et al., 2007, 2010; Apaydin et al., 2008; Chauhan et al., 2008 where authors are silent about conversion factor from barn to cm^2/g), they are less by a factor of $M_{L/M}/M_K$. $M_{L/M}$ always corresponds to a heavy element as compared to M_K. (With the σ_K^* values in barn in relation (6), the factor ($I_0 G a_{air}(e)\varepsilon(e)$ is in g^{-1} though it should be dimensionless). From relation (4), with the factor dimensions g^{-1}, though the $\sigma_{L/M}^*$ dimensions come out to be cm^2, i.e. in barn the values are less by the factor $M_{L/M}/M_K$).
3. The use of σ_K^* values in barn in relation (6) and evaluated $\sigma_{L/M}^*$ in cm^2/g from relation (4) (Rao et al., 1995, 1996; Durak and Ozdemir, 2001; Apaydin et al., 2005; Ozdemir, 2007; Küçükönder et al., 2008) is not justified as cm^2/g $\neq$ cm^2. Moreover, the values are to be multiplied by factor $1/M_K$.

In some cases, relations (3) and (6) (Kaya et al., 2001; Tirasoglu et al., 2001; Bastug et al., 2002) are employed for these evaluations where used and evaluated values are reported as barn; here the dimensions of $\sigma_{L/M}^*$ come as g.cm^2 and again the values are to be multiplied by factor $1/M_K$.

4. Conclusions

As has been shown here, in many publications there is confusion in using the cross-section in proper units and consequently the published, experimental results are higher by a factor ≥ 2 or less by factor $1/M_K$. Therefore, a careful re-inspection of those published data on XRF parameters is needed before using them.

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