INTENSITIES OF PRIMARY AND SECONDARY X-RAY SPECTRA

PHYSICS

1970

SovietRxiv

Abstract

Full Text

UDC 539.184:539.2

PHYSICS

A. T. STADNIKOV, A. P. NIKOLSKII

INTENSITIES OF PRIMARY AND SECONDARY X-RAY SPECTRA

(Presented by Academician G. V. Kurdyumov, 18 VII 1969)

1. Introduction. In studies of the electronic structure of a solid, there is at present a clearly expressed tendency toward combining various methods of exciting atoms to x-ray levels and studying the totality of the subsequent transitions, with the aim of obtaining more complete information on the properties of substances (^{1}). To compare the capabilities of different excitation methods, it is expedient to introduce characteristic parameters by which the corresponding conclusions could be drawn. In the method of x-ray spectral analysis, one such parameter is the number N_q^j, equal to the number of photons of the q-series emitted by the atoms of a sample into a solid angle of one steradian, on the average per one bombarding j-particle whose initial energy exceeds the ionization energy of the q-shell of the atoms.

The experimental determination of such, for example, physical quantities as the fluorescence yield (^{2}) and atomic ionization cross sections (^{3}) essentially reduces to measuring the parameter N_q^j, which is proportional to these quantities. The number N_q^j, called in (^{3}) the yield of characteristic photons (X-ray production), has been calculated in a relatively small energy range of ionizing particles—electrons (^{3}). In the present work an attempt is made to obtain more general analytical expressions for N_q^j, taking into account the material accumulated over the last 3 years ($^{4-10}$).

2. Algorithm of the solution. Let us consider the stationary distribution of a flux of ionizing j-particles incident on a massive homogeneous sample with initial energy E_0 at an angle θ_0 to its plane. The number dn of atoms of element A excited at the q-level in a layer dl g/cm^2, parallel to the surface of the sample and located at depth l g/cm^2, taking into account the processes of reflection, diffusion, and slowing down of the incident particles, is found from the expression for the relative excitation density $\Phi_j(l) = dn/dn_0$, whose dependence on l admits convenient analytical approximations (^{4,6,7}). The quantity

$$dn_0 = C\,\frac{N}{A}\,\frac{Q_q^j(E_0)\,dl}{\sin\theta_0} \tag{1}$$

is equal to the number of excited atoms of the element under consideration in the same layer, but isolated in space, i.e., placed in the same position without being surrounded by the body of the sample (7). The quantities dn and dn_0 are calculated on the average per one incident j-particle. In formula (1), N is Avogadro' s number; CN/A is the number of atoms of the element under consideration in 1 g of the sample; C is the mass concentration of this element; A is its atomic number; $Q_q^j(E_0)$ is its atomic excitation cross section at the q-level by j-particles with energy E_0.

Multiplying dn by $\omega_q p_{qi} \alpha_j \exp(-\chi l)/4\pi$ (where ω_q is the fluorescence yield of the q-series; p_{qi} is the fraction of photons of the $q \to i$ transition out of the total number of photons of this series; $\chi = \mu_m(\lambda_{qi}) \operatorname{cosec} \theta$; $\mu_m(\lambda_{qi})$ is the mass absorption coefficient in the sample for photons with wavelength λ_{qi}; θ is the takeoff angle of these photons, measured from–

measured from the plane of the sample, α_j is the correction for the increase in the intensity of the x-ray spectra under consideration due to the radiation of the sample accompanying the incident flux of j-particles) and integrating the result over dl, we find the value of the production of photons of the characteristic radiation of atoms of element A into a solid angle of 1 steradian from the entire massive sample:

$$N_q^j = \frac{C}{4\pi} \frac{N}{A} \omega_q p_{qi} \alpha_j Q_q^j(E_0) \int_0^\infty \frac{\Phi_j(l)}{\sin \theta_0} e^{-\chi l} \, dl. \tag{2}$$

Our specific problem is the calculation, by formula (2), of photon production when the sample is irradiated by electrons with energies $2 \div 150$ keV and by x-ray photons of the same energies.

3. Excitation of atoms by electron impact. Approximating the relative density $\Phi_e(l)$ of atoms excited by electrons by a Gaussian distribution (6), from formula (2) we find for a pure element A with atomic number Z the value of the production of characteristic-radiation photons by a normally incident electron with kinetic energy E_0:

$$N_q^e = \frac{1}{4\pi} \frac{N}{A} \omega_q p_{qi} Q_q^e(E_0) \frac{2a_e b_e}{1 + \chi b_e} f_0 \Phi_e(0); \tag{3}$$

$$b_e = 1.73 \cdot 10^{-5} \frac{A}{Z^{1/3}} \left(\frac{E_0^{1.8}}{1.8 \ln(174 E_0/Z)} - \frac{E_q^{1.8}}{1.8 \ln(174 E_q/Z)} \right) \text{ g/cm}^2; \tag{4}$$

$$f_0 = 0.633 e^{u^2} \left(1 + \frac{2}{\sqrt{\pi}} \int_0^u e^{-t^2} \, dt \right) (1.505 - 1.42u); \tag{5}$$

$$u = 0.357 - 0.7 \chi b_e, \tag{6}$$

where $Q_q^e(E_0)$ is the atomic cross section for excitation by an electron with energy E_0 of atom A to the q-level (^{4}); $\Phi_e(0)$ is the density of ionization of atoms A by electrons at the surface of the sample, determined from the graphs (^{7}); α_e is the correction for the increase in the intensity of the radiation under consideration due to the continuous and characteristic radiation of the sample (^{8}). The initial kinetic energy of the electron E_0 and the critical energy for excitation of atom A to the q-level, E_q, are expressed in formula (4) in kiloelectron-volts.

In the case where element A is dissolved in a sample with concentration C, and the bombarding electrons fall obliquely to the surface of the sample, corrections must be introduced into formula (3). The methods for introducing them have not been developed sufficiently fully, especially for light emitting elements (^{4}). Nevertheless, the value of N_q^e can be estimated. To this end we multiply the value (3) by C, take the parameters χ in formulas (3), (6) and Z, A in formula (4) with allowance for the composition of the matrix, and introduce a correction for the angle θ_0 similarly to how this was done in the calculations (^{9,11}). As a result we find that

$$N_q^e \approx \frac{C}{4\pi}\frac{N}{A}\omega_q p_{qi} Q_q^e(E_0)\frac{2a_e b_e f_0}{1+\chi b_e \sin\theta_0}\Phi_e(0). \tag{7}$$

Let us note that for any Z and Z_{matrix} in the energy range of the bombarding electrons under consideration, the quantity $b_e \approx 1/\sigma$, where $\sigma = 2.39 \cdot 10^5/(E_0^{3/2} - E_q^{3/2})$ cm^2/g is the Lenard coefficient (^{4,7}), and the product $f_0\Phi_e(0) \approx 1 \div 1.5$. Taking these equalities into account, the estimate of (7) is substantially simplified.

4. Excitation of atoms by x-ray photons. The relative density of excited atoms of a sample irradiated by a monochromatic beam of x-ray photons with energy E_0, deter-

is described by the exponential law of attenuation of the intensity of the incident beam (^{2,11}). Taking account of back reflection of photons, this density is equal to

$$\Phi_x(l) = \Phi_x(0)\exp(-l/b_x \sin\theta_0); \tag{8}$$

$$b_x = 1/\mu_m(\lambda), \qquad \lambda_0 = hc/E_0; \tag{9}$$

$$\Phi_x(0) = 1 + \eta_x \frac{\sin\theta_0}{\sin\theta_x}, \tag{10}$$

where h is Planck' s constant; c is the speed of light; η_x is the coefficient of back reflection of the bombarding photons; θ_x is the effective angle of this reflection, measured from the surface of the specimen.

Substituting function (8) into formula (2), we find the value of the yield of characteristic-radiation photons produced by a bombarding photon with energy E_0:

$$N_q^x = \frac{C}{4\pi}\frac{N}{A}\omega_{qp_{qi}} Q_q^x(E_0)\frac{a_{xb}x}{1+\chi b_x \sin\theta_0}\left(1+\eta_x\frac{\sin\theta_0}{\sin\theta_x}\right), \tag{11}$$

where $Q_q^x(E_0)$ is the cross section for excitation by a photon of an atom A to the q-level; a_x is the correction for the increase in the radiation intensity of atoms A by characteristic radiation of the specimen (8).

5. Conclusion. 1) Theoretical limits have been found for the intensities of primary and secondary spectra, determined respectively by the yields of X-ray photons of the characteristic radiation of specimen atoms into a solid angle of 1 steradian per 1 bombarding electron (3), (7) and photon (11).

2) A positive feature of the analysis of substances by primary spectra is the possibility of controlling the energy of the bombarding electrons by changing the magnitude of the accelerating voltage. The optimal regime for excitation of primary spectra corresponds to the plateau region of the spectrometer characteristic "accelerating voltage–counting rate of recorded pulses," where the influence of instability of the accelerating voltage on the spectrum intensity is minimal, and the photon yield has a maximum. The value of the energy of the bombarding electrons optimal for excitation of primary K-spectra, corresponding to reaching this plateau, is equal to the larger of the two quantities E_1 and E_2:

$$E_1 = \left(\frac{3\cdot 10^5 \sin\theta}{\mu_m(\lambda_{ki})\sin\theta_0}\right)^{2/8} \text{ keV}, \qquad E_2 = 6E_K,$$

where $\mu_m(\lambda_{ki})$ is expressed in cm^2/g, and E_K is the energy of the K-absorption edge.

3) The yield of photons of primary K-spectra of elements from Ti to Na, dissolved in small amounts in a filler with atomic number $Z_{\text{filler}} = 23 \div 28$ ($\chi \sim Z^{-17/3}$), decreases with decreasing atomic number Z of the dissolved emitter elements approximately in proportion to $Z^{3.5}$. This estimate was made from formula (7) under fulfillment of one of the conditions for the optimal regime of excitation of primary K-spectra formulated above, according to which the energy of the bombarding electrons is chosen equal to E_1, i.e., in the case considered, varies in proportion to $Z^{34/9}$.

4) The magnitude of the intensity of secondary spectra of light elements falls sharply with decreasing atomic number if the soft component of the ionizing X-radiation is filtered before it reaches the specimen (for example, by the material of the window of the X-ray tube).

In particular, the intensity of secondary K-spectra of light elements dissolved in small amounts in a filler with atomic number $Z_{\text{filler}} = 23 \div 28$ ($\chi \sim Z^{-17/3}$, $\chi b_x \sin\theta_0 \gg 1$), decreases with decreasing atomic number Z of the emitter elements in proportion to Z^{12}, i.e., by a factor of $4 \cdot 10^3$

when Z is decreased by a factor of two from Ti to Na, if in the beam of ionizing X-ray radiation the number of photons with energy $E_0 < 5$ keV is small compared with the number of harder photons. The estimate given above for the intensity $\approx Z^{12}$ was made according to formula (11) for $E_0 = \text{const} \gtrsim 5$ keV.

The sensitivity of analysis by the secondary K-spectra of elements from Ti to Na, according to the experimental data of work [12], also worsens approximately in proportion to Z^{12}, i.e., like the calculated value of the production of photons (11) of the characteristic radiation of these elements.

5) Comparison of the quantities (7) and (11), at optimal values of the energies of the bombarding electrons and photons and under equal geometrical conditions, shows that the maximum production of photons of the secondary K-spectra of elements heavier than carbon is higher than the maximum of the primary spectra.

All-Union Scientific Research Institute
for Automation of Ferrous Metallurgy
Moscow

Received
27 VI 1969

CITED LITERATURE

[1] International Symposium, *X-Ray Spectra and the Electronic Structure of Substances* (abstracts of reports), Kiev, 1968.
[2] A. Compton, S. Allison, *X-Rays. Theory and Experiment*, L.–M., 1941.
[3] M. Green, V. E. Cosslet, J. Phys. D, Ser. 2, 1, No. 4, 425 (1968).
[4] H. E. Bishop, J. Phys. D, Ser. 2, 1, No. 6, 673 (1968).
[5] J. Philibert, R. Tixier, J. Phys. D, Ser. 2, 1, No. 6, 685 (1968).
[6] C. A. Andersen, D. B. Wittry, J. Phys. D, Ser. 2, 1, No. 5, 529 (1968).
[7] A. Vignes, G. Dez, J. Phys. D, Ser. 2, 1, No. 10, 1309 (1968).
[8] T. Ichinokawa, Japan. Analyst, 15, No. 3, 302 (1966).
[9] V. P. Afonin, Izv. AN SSSR, ser. fiz., 31, No. 6, 1006 (1967).
[10] I. B. Borovskii, V. I. Rydnik, Izv. AN SSSR, ser. fiz., 31, No. 6, 1009 (1967).
[11] M. A. Blokhin, *Physics of X-Rays*, Moscow, 1967.
[12] Von Herm.-Jos. Kopineck, Rev. Univ. Mines, 17, No. 4, 214 (1961).

Note: Figure translations are in progress. See original paper for figures.

Source: Math-Net.Ru and CyberLeninka. Machine translation. Verify with the original.