Brazilian Journal of Physics
ISSN: 0103-9733
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Sociedade Brasileira de Física
Brasil

Czarnota, M.; Pajek, M.; Banás, D.; Dousse, J.-Cl.; Maillard, Y.-P.; Mauron, O.; Raboud, P. A.; Berset, M.; Chmielewska, D.; Rzadkiewicz, J.; Sujkowski, Z.; Hoszowska, J.; Slabkowska, K.; Polasik, M.
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Brazilian Journal of Physics, vol. 36, núm. 2B, june, 2006, pp. 546-549
Sociedade Brasileira de Física
São Paulo, Brasil

Multiple Ionization Effects in X-Ray Emission Induced by Heavy Ions

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Received on 29 July, 2005

The x-ray satellite structure of Pd $L\alpha_{1,2}(L_3M_{4,5})$ transition excited by an impact of O^{7+} and Ne^{6+} ions with energies 279 and 178 MeV, respectively, which were measured using a high-resolution von Hamos crystal spectrometer, is discussed in terms of the multi-configuration Dirac-Fock (MCDF) calculations. We demonstrate, by using the arguments of the general central limit theorem (GCLT), that a structure of complex M-shell satellites of Pd $L\alpha_{1,2}(M^{-m})$ transitions for a higher number of spectator vacancies ($m > 4$), which consists of hundreds of thousands of individual x-ray transitions as obtained from the MCDF calculations, can be well described by a single Voigtian profile. The Lorentzian width of such Voigtian line can be well modeled by using the results of the MCDF calculations for simpler configurations with a number of vacancies $m \leq 4$. This method allows one to describe realistically a complex structure of M-shell satellites, thus extending the applicability of the MCDF calculations, which are limited by an increasing complexity of numerical calculations.

Keywords: Multiple ionization; X-ray satellite structure; MCDF calculations

I. INTRODUCTION

The x-rays emitted from atoms multiply ionized by heavy ions exhibit, apart from the well known x-ray diagram lines, the satellite structure corresponding to different multi-vacancy configurations present at the moment of the x-ray emission. High-resolution measurements of excited x-ray satellites give thus access to study the structure of multi-vacancy configurations in atoms. However, in order to extract from such complicated spectra the x-ray transitions the structure of x-ray multiplets and their Lorentzian widths for a given multi-vacancy configuration as well as the experimental Gaussian broadening have to be known. This results from the fact that for heavy ion impact the x-ray spectra, containing x-ray satellites with up to several spectator vacancies in the inner-shells, become extremely complex and, consequently, cannot be fitted uniquely without performing the MCDF calculations of the structure of individual x-ray multiplets and realistic modelling of their widths. In this paper we discuss a new method of analysis of complex x-ray spectra which, using the general central limit theorem arguments, describes the complex x-ray satellites as the smooth Vogtian profile having known mean value and width, which can be obtained from MCDF calculations. This method, which is based on our earlier works [1, 2], is presently extended to high-resolution spectroscopy. An alternative approach of analysis of x-ray spectra emitted from multiply ionized atoms can be found in a recent work by Horvat et al. [3].

In this paper we discuss the M- and N-shell satellites of Pd $L\alpha_{1,2}(L_3M_{4,5})$ x-ray transitions excited by fast O^{7+} and Ne^{6+} ions [4], which were measured with high-resolution ($\sim$ 1 eV) using crystal diffraction spectrometer [5]. The measured x-ray spectra were compared with predictions of the multi-configuration Dirac-Fock (MCDF) calculations. The details concerning the MCDF calculations adopted here are described in Ref. [6]. In fact, the x-ray satellites of the $L\alpha_{1,2}(L_3M_{4,5})$ transitions which are dominated by a small number of M-shell satellites, as for instance for O^{7+} ion impact on palladium ($m \leq 4$), can be well reproduced by MCDF calculations (see Fig. 1). However, for more complex configurations with a higher number of spectator vacancies ($m > 4$) the MCDF calculations become too complex numerically to be performed in practice. This is the case of Ne^{6+} impact on palladium (see Fig. 2), for which up to $m = 7$ M-shell satellites have to be calculated in order to reproduce the measured x-ray spectrum of Pd $L\alpha_{1,2}(L_3M_{4,5})$. We demonstrate, by using the general central limit theorem arguments, that the M-shell satellites for a higher number of spectator vacancies ($m > 4$) can be approximated by a single Voigtian profile for which a mean energy and width can be obtained by extrapolating the MCDF calculations for configurations with a smaller number of spectator vacancies.

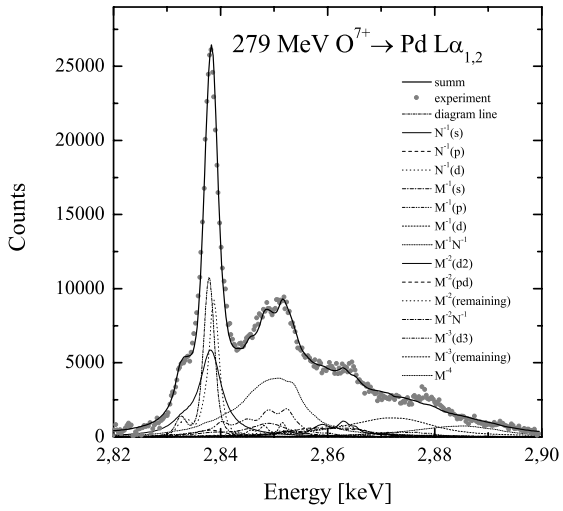

FIG. 1: Measured x-ray satellite structure for $L\alpha_{1,2}$ transition in palladium excited by 279 MeV O^{7+} ions. The data are compared with the predictions of the MCDF calculations including up to $m = 4$ spectator vacancies in the M- and N-shells. The individual components of the calculated spectrum are marked in the figure.

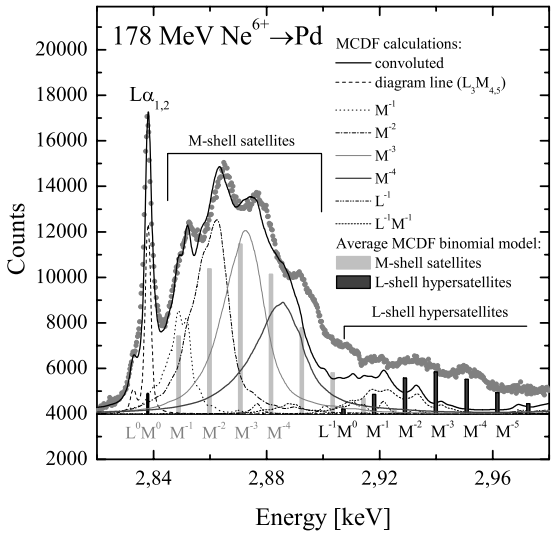

FIG. 2: Measured x-ray satellite structure for $L\alpha_{1,2}$ transition in palladium excited by 178 MeV Ne^{6+} ions. The data are compared with the predictions of the MCDF calculations including up to $m = 4$ spectator vacancies in the M- and N-shells and the average MCDF binomial model indicating the importance of configurations with up to $m = 8$ vacancies in the M-shell as well as the L-shell hypersatellite structure.

II. EXPERIMENT

The high-resolution measurements of the M- and N-shell satellites of Pd $L\alpha_{1,2}(L_3M_{4,5})$ x-ray transitions excited by fast O^{7+} and Ne^{6+} ions have been performed [8] at the Philips cyclotron in the Paul Scherrer Institute (PSI) in Villigen, Switzerland, using a von Hamos high-resolution diffraction spectrometer [5]. The x-ray spectra of $L\alpha_{1,2}(L_3M_{4,5})$ transitions were excited by O^{7+} and Ne^{6+} ion beams of energies 279 and 178 MeV, respectively, bombarding thin metallic palladium foils. The x-rays were measured by means of a high-resolution von Hamos spectrometer [5] with a precision of about 1 eV for studied Pd L-x-rays ($\sim$ 3 keV), including an experimental Gaussian resolution of about 0.7 eV. The von Hamos spectrometer was equipped with a quartz $(1\bar{1}1)$ crystal curved with a radius of 25.4 cm. The x-rays were measured with the CCD detector covering in one setting the x-ray energy range of about 50 eV. Consequently, the x-ray spectra of Pd $L\alpha_{1,2}(L_3M_{4,5})$ transitions were measured for several settings of the spectrometer. The energy calibration of the spectrometer has been performed by measuring well resolved $K\alpha_{1,2}$ x-ray lines of vanadium excited by photons from x-ray tube with Cr anode.

III. RESULTS AND DISCUSSION

In order to interpret quantitatively the measured x-ray satellite structure of Pd $L\alpha_{1,2}(L_3M_{4,5})$ transitions excited by Ne^{6+} ions of energy 178 MeV, MCDF calculations involving up to seven M-shell spectator vacancies are needed. However, the MCDF calculations for multi-vacancy Pd $L\alpha_{1,2}$ (M^{-m}) configurations become, in practice, numerically intractable for $m > 4$. For instance, the MCDF calculations for palladium for M^{-4} configuration contain 244953 transitions (see Fig. 3) and for mixed $M^{-1}N^{-2}$ configuration 268210 transitions. Such numerical limitation of the applicability of the MCDF calculations asks for developing of alternative approximate methods to treat the complex satellite structures of x-rays excited in ion-atom collisions.

Following the idea presented in our earlier works (see Refs. [1] and [2]) on multiple ionization effects in ion-induced x-ray spectra we suggest that the x-ray profile for complex x-ray transitions can be well approximated by an effective single profile resulting from a convolution of natural Lorentzian and experimental Gaussian widths applied to the calculated MCDF x-ray multiplets consisting of large number of transitions. This observation is based on the firm ground of the general central limit theorem (see Ref. [7]) suggesting a Voigtian type profile as the limiting distribution in our case.

In order to verify this idea, the calculated MCDF structure of x-ray transitions for Pd $L\alpha_{1,2}$ (M^{-m}) configuration, convoluted with natural Lorentzian widths of *individual transitions*, assumed to scale approximately with a number of spectator vacancies m as $\Gamma(m) = \Gamma(0) + 2\Gamma_{spec} \cdot m$, and experimental Gaussian widths of about 0.7 eV, are shown in Fig. 4. The effective widths of the *resulting* Voigtian profiles for complex x-ray multiplets are expected to follow approximately a simple scaling rule, namely,

$$\Gamma(m) = \Gamma_M(0) + \alpha m + \beta\sqrt{m} \qquad (1)$$

where α and β are constants which can be fitted for a calcu-

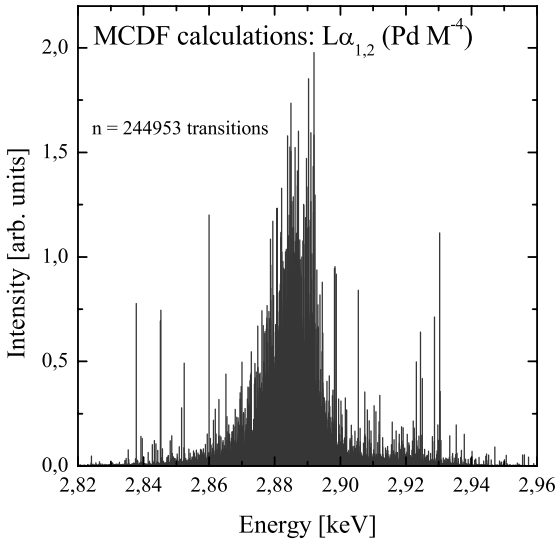

FIG. 3: The structure of Pd $L\alpha_{1,2}(M^{-4})$ x-ray transitions obtained by using the MCDF calculations.

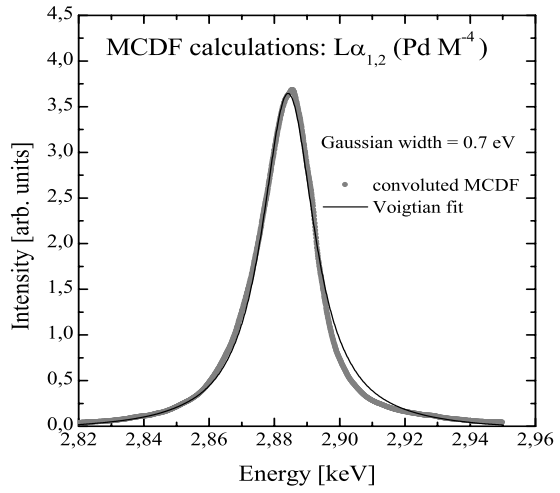

FIG. 4: A profile of $L\alpha_{1,2}(M^{-4})$ x-ray transitions, as obtained by convolution of calculated MCDF transitions with natural Lorentzian (see text) and experimental Gaussian widths, fitted by a single Voigtian profile. Note the smooth shape of the calculated (MCDF) profile and the reasonable good fit by a Voigtian.

lated MCDF configuration with a smaller number of spectator vacancies, $m \leq 4$ in our case. This formula, which uses once more the arguments of the GCLT theorem, has been derived by summing up the natural width $\Gamma(m)$ of the Lorentzian distribution of x-ray transition energy and the width of the binomial distribution of a number of vacancies randomly distributed in the M-shell. In fact, the variance of the binomial distribution $\sigma^2(m) = N_M p_M(1-p_M)$, where N_M is a number of electrons in the M-shell, scales for $p_M = m/M \ll 1$ as $\sigma^2(m) \propto m$ yielding the following approximate estimate for a width: $\Gamma_{bin}(m) \propto \sqrt{m}$.

The fitted effective widths of x-ray transitions for M^{-m} configurations, shown in Fig. 5, fully justify the model assumed. Consequently, such a parameterization of Voigtian widths for complex multi-vacancy configurations, combined with a known linear parameterization of their mean energies adopted in the average MCDF binomial model (Ref. [6]) of x-ray satellite structure, allows one to describe in a realistic way the complex x-ray spectra excited by heavy ions, which include much more spectator vacancies than can be treated numerically in an exact way using the MCDF calculations.

The present findings open a possibility to describe a complex satellite structure of Pd $L\alpha_{1,2}(L_3M_{4,5})$ transitions such as in the discussed x-ray spectra excited by Ne^{6+} ions of energy 178 MeV exhibiting M- and N-shell satellites. However, a final interpretation of such x-ray spectra needs further MCDF calculations for the observed L-shell hypersatellite structure overlapping with M-shell satellites. Such MCDF calculations of L-shell hypersatellites are in progress.

IV. CONCLUSIONS

A novel approximate description of x-ray spectra for complex multi-vacancy M^{-m} configurations has been proposed, which is based on the general central limit theorem. The calculated profiles of $L\alpha_{1,2}$ (M^{-m}) x-ray transitions in palladium are well described by the proposed model. Complex multi-vacancy configurations, involving up to about ten spectator

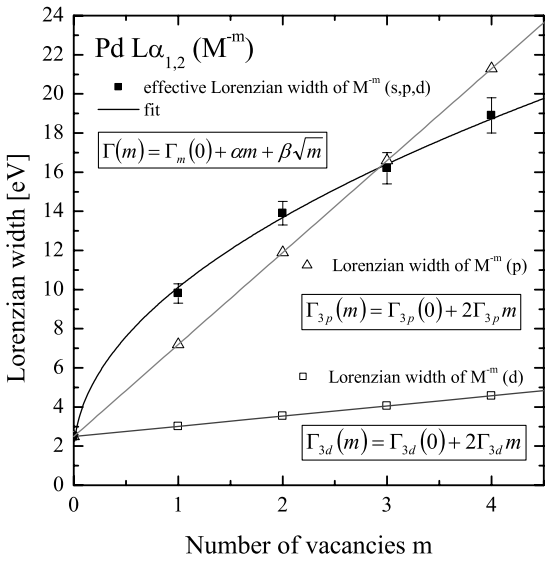

FIG. 5: Fitted effective Lorentzian widths of Pd $L\alpha_{1,2}(M^{-m})$ MCDF x-ray transitions for spectator vacancies in s-, p-, and d-states, which are well fitted by the approximate formula $\Gamma(m) = \Gamma_M(0) + \alpha m + \beta\sqrt{m}$. Assumed natural widths for M^{-m} vacancy configurations with vacancies in 3p and 3d states are also shown in the figure.

vacancies, can be treated within this approach, which significantly extends the applicability of the MCDF calculations for describing multiple ionization effects in x-ray spectra excited by heavy ions.

Acknowledgments

This work was supported by the Polish State Committee for Scientific Research under the Grant No. 1P0301326 and the Swiss National Science Foundation.

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