International Journal of Scientific Research in Science and Technology
Print ISSN: 2395-6011 | Online ISSN: 2395-602X (www.ijsrst.com)
doi :https://doi.org/10.32628/IJSRST52310352

Plasmon Effects in Non-Diagram X- Ray Spectra of Calcium (Ca) and Cobalt (Co)

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ARTICLEINFO

Article History:

Accepted: 05 May 2023
Published: 20 May 2023

Publication Issue

Volume 10, Issue 3
May-June-2023

Page Number

315-319

ABSTRACT

In recent years the whole area of high energy excitations in solid has flourished well, both experimentally and theoretically. Their spectroscopy and theoretical understanding have important implications for the knowledge of the structure and properties of materials, both in bulk and near the surface. The theory used in the present work, relates to origin of Non-diagram X-ray spectra in various excitation processes where a deep as well as the surface electron is excited. The specific contributions of the intrinsic as well as the extrinsic 'Plasmon-coupling' processes have been obtained theoretically in terms of "Non-diagram-to-parent-diagram X-ray line yield ratios" for the high energy plasmon satellite profiles in the X-ray line spectra of $K\alpha L^{(0)}$ main lines in Calcium (Ca) and Cobalt (Co) by extending the Bohm-Pines Hamiltonian and using many body theory. It has been shown that the high-energy X-ray satellite line shapes of Calcium (Ca) and Cobalt (Co) observed by Mauron and Dousse are due to the Plasmon Oscillations. The theoretically calculated results have been probed by comparing to the relative satellite yields obtained by Mauron and Dousse and are found to agree well with their experimentally observed values.

KEY-WORDS: Plasmon Satellites, Bulk Plasmon, Surface Plasmon, Plasmon Coupling

I. INTRODUCTION

Valence electrons in metal can take part in quantized collective oscillations known as Plasmons. The circumstances and extent to which Plasmons are involved in the production of X-ray satellites have been a topic of extensive experimental and theoretical investigations [1-24]. Satellites on the low energy side of X-ray emission spectra have been shown [17-18] to be associated with surface or bulk plasmon creation. In filing a vacancy in the core level of atoms, the de-excitation energy may be shared between a photon (which is seen as a low energy satellite) and a surface or bulk plasmon which is created in material. It is possible that de-excitation energy may be augmented by the surface or bulk plasmon energy, forming a satellite at energy higher than the parent - diagram X-ray line [12,16-18]. In this case, high energy electrons incident on the material would create both, the core level energy electrons excitations and Surface($\hbar\omega_s$) or Bulk ($\hbar\omega_P$) plasmons.

The theory [18] used in present work, relates to the origin of non- diagram X-ray Spectra in various excitation processes where deep as well as surface electron is excited. The specific contributions of the intrinsic as well as the extrinsic 'Plasmon-coupling' processes have been obtained theoretically in terms of "Non-diagram-to-parent-diagram X-ray line yield ratios" for the high energy plasmon satellite profiles in the X-ray line spectra of $K_\alpha L^{(0)}$ main lines in Calcium (Ca) and Cobalt (Co) by extending the Bohm-Pines Hamiltonian and using many body theory [19]. It has been shown that the high-energy X-ray satellite line shapes of Calcium (Ca) and Cobalt (Co) observed by Mauron and Dousse [20] are due to the Plasmon Oscillations. The theoretically calculated results have been probed by comparing to the relative satellite yields obtained by Mauron and Dousse [20] and are found to agree well with their experimentally observed values.

II. EXPRESSION FOR NON-DIAGRAM-TO-PARENT-DIAGRAM-X-RAY LINE YIELD RATIOS (RELATIVE INTENSITIES) IN X-RAY EMISSION SPECTRA

The transition probability per unit time [18] for the Interaction Hamiltonian $H_{2\hbar\omega_P}$:

$$H_{add} = H_{2\hbar\omega_P} = \frac{1}{2}\Sigma_{p,k',k<k_c}\frac{1}{(2\hbar\omega_P)^2}\frac{V(\bar{p}+\bar{k}+\bar{k'})M_k M_{k'}}{\left[2\omega_P - \frac{(\bar{k}+\bar{k'}).\bar{p}_i}{m} - \frac{\hbar\,(\bar{k}+\bar{k'})^2}{2m}\right]}$$

is given by $\sigma = \left(\frac{2\pi}{\hbar}\right) < f\ |H_{2\hbar\omega_P}| i >^2 \rho(E)$

The relative transition probability or relative intensity may be expressed as:

$$\frac{I_{2\hbar\omega_P(sat)}(E_P)}{I_0(E_P)} = \frac{1}{(4\hbar\omega_P)^2}\frac{1}{(2\pi)^3} \times \left\{\int_0^{k_c}\int_{-1}^{+1} 2k^2\,dk\,d(\cos\theta)\frac{{M_k}^2{M_{k'}}^2}{\left[2\omega_P - \frac{(\bar{k}+\bar{k'}).\bar{p}_i}{m} + \frac{\hbar\,(\bar{k}+\bar{k'})^2}{2m}\right]}\right\}$$

The relative intensity $\frac{I}{I_0}$ of bulk plasmon satellite profiles is expressed by simplifying this equation.

The matrix element defining simultaneous X-ray photon emission (photoemission) and surface plasmon absorption (loss feature) with momentum ħk when a valence electron with momentum p falls into a deep level may be written as:

$$< f\,|E.M."\_\,|i > = \left\{\frac{1}{4\hbar\omega_P}\right\}^{1/2} V(\bar{p}+\bar{k})M_k\left\{\frac{\frac{\hbar\bar{k}.\bar{p}}{m} - \frac{\hbar k^2}{2m}}{\frac{\omega_P}{\sqrt{2}} - \frac{\hbar\bar{k}.\bar{p}}{\sqrt{2}M} + \frac{\hbar k^2}{2\sqrt{2}M}}\right\}$$

If we suppose that V(p) does not depend upon p, then the relative transition probability or relative intensity may be expressed as

$$\frac{I_{sat}(E_P)}{I_0(E_P)} = \left(\frac{1}{4\hbar\omega_P}\right)\frac{1}{(2\pi)^3}\int_0^{k_c}\int_{-1}^{+1} 2\pi k^2 dk\,d(\cos\theta)\left\{\frac{\frac{\hbar\bar{k}.\bar{p}}{m} - \frac{\hbar k^2}{2m}}{\frac{\omega_P}{\sqrt{2}} - \frac{\hbar\bar{k}.\bar{p}}{\sqrt{2}M} + \frac{\hbar k^2}{2\sqrt{2}M}}\right\}{M_k}^2$$

The relative intensity $\frac{I}{I_0}$ of surface plasmon satellite profiles is expressed by simplifying this equation.

In summary, the strength I/I_o of the nth plasmon loss feature (if the main line is normalized to unit strength, here I_o) is equal to the coefficient of x^n in the expansion [21] of $e^{\beta x}[(1-\alpha x)^{-1}]$, - (1)

where the exponential represents the 'intrinsic' effect and the quantity in brackets is the 'extrinsic' effect.

Therefore, the combined effects of intrinsic and extrinsic **"Plasmon Coupling Processes"** in terms of the relative intensity of the high energy plasmon satellites in the X- ray line spectra of Calcium (Ca) and Cobalt (Co) is obtained [22] as:

$\frac{I}{I_0} = \alpha^n \sum_{m=0}^{n} \frac{(\beta/\alpha)^m}{m!}$ (2)

The value of β is taken as

$\beta = 0.12\ r_s$, (3)

and the value of α (= K_C/K_F) is taken as

$\alpha = 0.47\ r_s^{1/2}$. (4)

Again, r_s (dimensionless parameter) is the inter-electronic spacing in units of the Bohr radius and may be expressed as

$r_s = (47.11/\hbar\omega_p)^{2/3}$ for bulk plasmon,

& $r_s = (47.11/\hbar\omega_s)^{2/3}$ for surface plasmon.

The bulk plasmon energy of a metal may be expressed as

$\hbar\omega_p = 28.8\ (Z'\sigma/W)^{1/2}$

Where Z' is the effective number of electrons participating in plasma oscillations (number of conduction or valence band electrons), σ is the specific gravity and W is the molecular weight.

As usual, the surface plasmon energy is $\hbar\omega_s = \hbar\omega_p/\sqrt{2}$ (if the geometry of the specimen is plane).

III.RESULTS

(i) For CALCUIM (Ca)

Table-1 Energy - Separation (ΔE) of High Energy Satellites of Calcium (Ca)for $K_\alpha L^{(0)}$ X- Ray Main Line

Sl. No.	$K_\alpha L^{(1)}$ Satellites of Ca	Z'	σ	W	Author's calc. values	Observed energy-separation by Mauron and Dousse (ΔE), eV
1.	Satellite Line (I): 3712eV	2	4.58	40.078	19.6 eV ($2\hbar\omega_s$)	20.0
2	Satellite Line (II): 3716eV	2	4.58	40.078	23.6 eV ($\hbar\omega_p + \hbar\omega_s$)	24.0

* $K_\alpha L^{(0)}$ **Main Line of Ca : 3692 eV**

Table-2 Relative Intensity 'I/Io' of High Energy Plasmon Satellites $K_\alpha L^{(1)}$ of Calcium (Ca)for $K_\alpha L^{(0)}$ X-Ray Main Line

Sl. No.	$K_\alpha L^{(1)}$ Satellites of Ca	$r_s = \left(\frac{47.11}{\Delta E^{eV}}\right)^{2/3}$	$\beta = 0.12 r_s$	$\alpha = 0.47(r_s)^{1/2}$	Intensity Assignment "I/I_0"	Theoretical value of "I/I_0" in Present Work	Observed value of "I/I_0" by Mauron and Dousse
1.	Satellite Line (I): 3712eV	1.794	0.2153	0.6296	$\frac{\beta^2}{4\alpha}$	0.0261	0.0256
2	Satellite Line (II): 3716eV	1.585	0.1903	0.5918	$\frac{\beta^2}{2\alpha}$	0.031	0.034

*$K_\alpha L^{(0)}$ **Main Line of Ca : 3692 eV**

(ii) For COBALT (Co)

Table-1 Energy - Separation (ΔE) of High-Energy Satellite of Cobalt (Co) for $K_\alpha L^{(0)}$ X- Ray Main Line

Sl. No.	Satellite of Co	Z'	Σ	W	Author's calc. value	Observed energy-separation by Mauron and Dousse (ΔE), eV
1.	$K_\alpha L^{(1)}$ Satellite Line : 6960eV $K_\alpha L^{(0)}$ Main Line: 6931eV	3	4.8	58.933195	28.5 eV ($2\hbar\omega_p$)	29.0

Table-2 Relative Intensity 'I/Io' of High Energy Plasmon Satellite $K_\alpha L^{(1)}$ of Cobalt (Co) for $K_\alpha L^{(0)}$ X-Ray Main Line

Sl. No.	$K_\alpha L^{(1)}$ Satellite of Co	$r_s = \left(\frac{47.11}{\Delta E^{eV}}\right)^{2/3}$	$\beta = 0.12 r_s$	$\alpha = 0.47 (r_s)^{1/2}$	Intensity Assignment "I/I_0"	Theoretical value of "I/I_0" in Present Work	Observed value of "I/I_0" by Mauron and Dousse
1.	$K_\alpha L^{(1)}$ Satellite Line : 6960eV $K_\alpha L^{(0)}$ Main Line : 6931eV	1.3980	0.168	0.556	$\frac{\beta^2}{4\alpha}$	0.0127	0.0119

IV. CONCLUSION

Thus, one can safely assume, from the energy-separation as well as from the relative intensity point of view that the high energy satellite profiles observed by Mauron and Dousse [20] in the X-ray line spectra of $K_\alpha L^{(0)}$ main lines of Calcium (Ca) and Cobalt (Co) are due to Bulk and Surface Plasmon Oscillations.

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