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Plasmons in Non-Diagram X-ray Spectra of Scandium and Titanium Compounds

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ABSTRACT

In recent years the whole area of high-energy excitations in solids 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 the bulk and near the surface. The theory used in the present work relates to the origin of Non-diagram X-ray spectra in various excitation processes where a deep, as well as the surface electron, is excited. By extending the Bohm-Pines Hamiltonian and utilizing many-body theory, the specific contributions of intrinsic as well as 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 $2P_{1/2}$ main line in compounds of Scandium and Titanium. It has been shown that the high energy X-ray satellite line shapes of Scandium and Titanium compounds observed by de Boer et al. are due to the Plasmon Oscillations. The theoretically calculated results have been probed by comparing them to the relative satellite yields obtained by de Boer et al. and are found to agree well with their experimentally observed values than their calculated values.

Keywords :- Bulk Plasmon, Surface Plasmon, Plasmon satellites, Critical Wave -Vector, Plasmon Field.

I. INTRODUCTION

Plasma longitudinal waves are a form of elementary excitation that is correlated to the collective motion of weakly valence electrons to the positive ion crystal lattice in solids. Plasmons are the quanta of these waves with energy $E_p = \hbar\omega_p$ [1]. Plasmons are hence quantized oscillations of collectively arranged electrons in the valence bonds of semiconductors, metal conduction bands, and dielectrics [2]. The bulk plasmon and surface plasmon ($E_s = \hbar\omega_s = \hbar\omega_p/\sqrt{2}$) are the two primary kinds of plasmons, which are separated based on the manner and conditions of excitation [2].

In semiconductors and solids, bulk plasmons are longitudinal oscillation modes of the electron gas and are defined by the condition $\varepsilon = 0$, where ε is the bulk dielectric function. The surface plasmon is an oscillating sheet of charge that is positioned at the surface although its energy is constrained by the bulk properties $\varepsilon = -1$. Various experimental and theoretical studies have focused on the condition and extent to which Plasmons are engaged in the creation of X-ray satellites [1-21].

In the characteristic X-ray emission spectra, "X-ray satellites" (Secondary Emission lines) or "Non-diagrams lines" are relatively faint lines that are frequently seen adjacent to the "Main emission or diagram lines". Loss Energy satellites (LES) are satellites seen on lower energy sides of the main lines and High Energy Satellites (HES) are satellites seen on higher energy sides of the main lines.

In addition to the importance of solving these issues for X-ray spectroscopy, a careful study of satellites appears to allow one to obtain valuable information on the ionization mechanism of the inner shells of atoms, on the phenomena accompanying this process, as well as on the behaviour of an electron in a solid. Many classes of X-ray satellites have natures and properties that, unlike those of the main lines, are currently unknown. In this work, an effort is being made to examine the characteristics and provide an explanation for the nature of some types of satellites. This effort is based on the idea that valence electrons of atoms in solids undergo PLASMA OSCILLATIONS when the number of inner electrons changes, leading to the creation of vacancies in the inner shells of atoms [23].

Bulk plasmon generation has been attributed to satellites on the low-energy side of the X-ray emission spectrum. The de-excitation energy may be shared by a photon (which is viewed as a low-energy satellite) and a bulk plasmon that is produced in the material while filling a hole in the core level of atoms. Bulk plasmon energy that forms a satellite at an energy higher than the parent-diagram X-ray line could potentially increase the de-excitation energy [4]. Core-level electron excitation and bulk plasmon would both be produced in this scenario by a high-energy electron impinge on the material. The possibility of observing a plasmon satellite at an energy distance of $\hbar\omega_p/\sqrt{2}$ (if the specimen's geometry is plane) from the main line has been investigated in several experiments.

The various factors that influence the strength of non-diagram X-ray emission's plasmon excitation to enhance the field of plasmon physics (line yield ratio). As a result of the valence electron being drawn to screen the core hole by the sudden change in potential, the intrinsic plasmon is excited [5–6]. Additionally, a quantum interference process between the intrinsic and extrinsic plasmons results in interference. the interaction between a localized core hole (intrinsic) and a traversing electron (extrinsic), where the virtual plasmon produced by one is absorbed by the other. The theory [7] that will be applied in this study relates to the emergence of non-diagram X-ray spectra in a variety of excitation processes when both a deep and a surface electron are stimulated. By extending the Bohm-Pines Hamiltonian and utilizing the many-body theory [8] for the bulk plasmon and the surface plasmon satellites structures in the X-ray line spectra of metal and semiconductor, the specific contribution of intrinsic as well as extrinsic "Plasmon-Coupling Processes" is theoretically obtained in terms of "NON-DIAGRAM-TO-PARENT-DIAGRAM X-RAY LINE YIELD RATIO.

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

The transition probability per unit time [7-8] for the Interaction Hamiltonian $H_{2\hbar\omega_P}$: $H_{add} = H_{2\hbar\omega_P} = \frac{1}{2}\sum_{p,k',k<k_c} \frac{1}{(2\hbar\omega_P)^2} \frac{V(\bar{p}+\bar{k}+\bar{k'})M_k M_{k'}}{\left[2\omega_P - \frac{(\bar{k}+\bar{k'}).\bar{p}_i}{m} - \frac{\hbar(\bar{k}+\bar{k'})^2}{2m}\right]}$

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

The relative transition probability or relative intensity can 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 de level can be represented 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 $V(\overline{p})$ does not depend upon p, then the relative transition probability or relative intensity can 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 [9] of

$$e^{\beta x}[(1-\alpha x)^{-1}], \qquad - (1)$$

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 for high energy plasmon satellites in X- ray line spectra of Scandium and Titanium compounds obtained [10] as:

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

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

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

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

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

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

Table-1

Energy - Separation (ΔE) for High Energy Plasmon Satellites in X- ray Line Spectra of $2P_{1/2}$ Main Line of Scandium and Titanium compounds

Sl. No.	Compounds	Z'	σ	W	Author's calc. Values		Observed energy-separation by de Boer et al. (ΔE), eV
					$\Delta E=\hbar\omega_p$eV	$\Delta E=\hbar\omega_s$eV	
1.	ScF_3	6	--	101.93	*		12.3
2.	TiF_4	8	2.79	123.89	12.30		13.40
3.	K_2TiF_3	---	---	555.50	*	--	7.30
4.	ScI_3	6	--	--	*	.	7.40
5.	TiI_4	8	4.30	555.50	7.20	.	7.3
6.	$ScBr_3$	6	3.91	284.85	8.30	.	8.6
7	$TiBr_4$	8	2.60	367.54	6.85		8.70
8	$ScCl_3$	6	2.39	151.47	8.9		9.60
9	$TiCl_4$	8	2.06	189.70	8.50		9.60
10	Sc_2O_3	12	3.86	138.20	16.67	11.80	11.20
11	TiO_2	8	4.26	79.90	18.80	13.30	13.40

* Could not be calculated due to non-availability of constants.

Table-2

Relative Intensity 'I/Io' of High Energy Plasmon Satellites in X- ray Line Spectra of $2P_{1/2}$ Main Line of Scandium and Titanium Compounds

Sl. No.	Compounds	$r_s = \left(\frac{47.11}{\Delta E^{eV}}\right)^{2/3}$	$\beta = 0.12 r_s$	$\alpha = 0.47 (r_s)^{1/2}$	Intensity Assignment "I/I_0"	I/I_0 In Present Work	I/I_0 by de Boer *et.al*	
						Calc.	Obs. as $I_{1/2}$	Calc. as $I_{1/2}$

1.	ScF_3	2.426	0.2911	0.7321	$\beta + \frac{\beta^2}{2\alpha}$	0.36	0.35	0.25
2.	TiF_4	2.426	0.2911	0.7321	$\beta + \frac{\beta^2}{2\alpha}$	0.35	0.43	0.17
3.	K_2TiF_3	2.227	0.2672	0.7014	$\beta + \frac{\beta^2}{2\alpha}$	0.32	0.30	0.32
4.	ScI_3	3.396	0.4075	0.8861	$\frac{\beta^2}{2\alpha} + \frac{\beta^2}{6\alpha^2}$	0.11	0.10	0.32
5.	TiI_4	3.460	0.4140	0.8730	$\frac{\beta^2}{2\alpha} + \frac{\beta^2}{6\alpha^2}$	0.11	0.25	0.44
6.	$ScBr_3$	3.145	0.3774	0.8335	β	0.38	0.30	0.25
7.	$TiBr_4$	3.570	0.4284	0.8880	$\frac{\beta^2}{6\alpha^2}$	0.02	0.04	0.34
8.	$ScCl_3$	3.003	0.3604	0.8145	$\beta + \frac{\beta^2}{6\alpha^2}$	0.37	0.40	0.22
9.	$TiCl_4$	3.096	0.3715	0.8270	$\beta + \frac{\beta^2}{6\alpha^2}$	0.38	0.41	0.30
10.	Sc_2O_3	2.493	0.2992	0.7421	$\beta + \frac{\beta^2}{2\alpha} + \frac{\beta^2}{6\alpha^2}$	0.37	0.40	0.29
11.	TiO_2	2.304	0.2766	0.7134	$\beta + \frac{\beta^2}{2\alpha} + \frac{\beta^2}{6\alpha^2}$	0.34	0.40	0.30

IV. CONCLUSION

Therefore, it is reasonable to believe that the high-energy Satellite profiles found in the $2P_{1/2}$ main line X-ray Spectra of Scandium and Titanium Compounds by de Boer et al. [24] are caused by Bulk and Surface Plasmon Oscillations based on the energy-separation as well as the relative intensity point of view.

REFERENCES

[1]. D. Pines, Elementary Excitations in Solids; CRC Press: New York, NY, USA, 1963.

[2]. J. M. Ziman, Principles of the Theory of Solids; Cambridge University Press: Cambridge, UK, 1964, 405p.

[3]. H. Rather, Surface plasma oscillations and their applications (A Review), Phys. Thin Films, 1977, 12, 154.

[4]. S. Hafner, Photoelectron Spectroscopy, Solid State Science Series, Vol.82, Springer-Verlag, 1995 (Chapter 3 and references there in).

[5]. C. Biswas et al., Phys. Rev. B67, (2003) 165416.

[6]. A.M. Bradshaw et al., J Phys. C. Solid State Phys. 7, (1974) 4503.

[7]. D.C. Langreth, in Collective Properties of Physical Systems, edited by B. Lundquist and S. Lundquist, Academic Press, New York (1974).
[8]. O.K. Harsh, J. Phys. Chem. Solids 58, N9, (1997) 1433.
[9]. J.J. Chang and D.C. Langreth, Phys. Rev. B8, (1973) 4638.
[10]. W.J. Pardee et al., Phys. Rev. B11, (1975) 3614.
[11]. S.P. Singh et al., Indian J. Phys. 85, N12, (2011) 1897.
[12]. Alok Mishra et. al., IJERA2, N2, (2012) 115-118.
[13]. M. Guzzo et al., Eur. Phys. J.B, (2012) 85:326.
[14]. L.K. Dwivedi, in Active and Smart Materials, edited by D.K. Dwivedi and B.K. Pandey, Excel India Press, New Delhi, (2012) 151-153.
[15]. L.K. Dwivedi, in Materials Science and Technology, edited by D.K. Dwivedi and B.K. Pandey, Victorious Publishers, Delhi, (2014) 138-140.
[16]. L.K. Dwivedi, in Proceedings of National Conference on “Recent Advances in Chemical and Materials Science (NCRACMS-15)”, MMMUT, Gorakhpur, U.P., (23-24 Feb., 2015) 64-65.
[17]. L.K. Dwivedi, Education Times (UGC No. 62976), Vol. IX, No. 11, (2018) 114-116.
[18]. L.K. Dwivedi, Edu World (UGC No.-62981), Vol. XII, No. 21, (2018) 81-85.
[19]. L.K. Dwivedi, Education Times (UGC No. 62976), Vol. IX, No.13, (2018) 9-11.
[20]. L.K. Dwivedi, Education Times (UGC No. 64512), Vol. IX, No.11, (2018) 13-17.
[21]. L.K. Dwivedi and Vipin Sharma, in Proceedings of International Conference on “Materials Science and Spectroscopy (ICMSS-21)”, MUIT, Lucknow, U.P., (Sept. 22-24., 2021) 77.
[22]. K.S. Srivastava et.al. Ind. Jour. of pure and Applied Phys. 34 (1995) 190.
[23]. L.G. Parratt, Rev. Mod. Phy. 31, (1959) 616.
[24]. D.K.G. de Boer et.al., Phy. Rev. B20, (1984) 4401.

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