Relative intensities of low-energy plasmon satellites in x-ray emission spectra of Li, Be, and Na

K. S. Srivastava, S. P. Singh, and R. L. Shrivastava

Department of Physics, K. N. Govt. Postgraduate College, Gyanpur, Varanasi, U. P., India

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We have calculated the relative intensities of low-energy plasmon satellites in the soft-x-ray emission spectra of lithium, beryllium, and sodium as 0.013, 0.0039, and 0.02, respectively. These values are in fair agreement with the observed values of Arakawa *et al.*

Ferrell[1] and Nozières and Pines[2] pointed out for the first time that plasma oscillations in solids can complicate the structure of the x-ray emission spectra, giving rise to some weak lines toward the low-energy side of the parent band. These weak lines are known as low-energy plasmon satellites. These satellites have been observed in aluminum, magnesium, and sodium by Rooke[3] and in beryllium by Watson *et al.*[4] Brouers[5] and Glick and Longe[6] have worked out theoretically the origin of low-energy plasmon satellites. These plasmon satellites are obtained when a valence electron before filling up the vacancy in the inner shell excites a plasmon. The energy of the emitted x-ray photon will be less by an amount of energy $\hbar\omega_p$ which has been used up in exciting the plasmon.

Recently Arakawa and Williams[7] have observed the low-energy satellites in the x-ray emission spectra of lithium, beryllium, and sodium at energy separations of 7, 18.5, and 5.5 eV, respectively, from the main band. They have claimed these low-energy satellites as due to volume plasmon creation merely on the basis of correspondence between the above energy separations and the characteristic energy-loss values reported by Kunz[8] (7.12 eV in Li), Sueoka[9] (18.7 eV in Be), Powell[10] (19 eV in Be), and Swan[11] (5.58 eV in Na). In the present paper, we have theoretically calculated the relative intensities of low-energy satellites of Li, Be, and Na and compared the results with experimentally observed[12] values of Arakawa and Williams.[7]

Following Brouers,[5] the model Hamiltonian which describes the interaction of electrons, the presence of a localized level vacancy, and its interaction with the electron gas followed by the x-ray emission in a system is expressed as

$$H = H_0 + H_{\rm EM}, \qquad (1)$$

where

$$H_0 = \frac{1}{2m}\sum_{\vec{p}} p^2 C^\dagger_{\vec{p}} C_{\vec{p}} + \frac{1}{2}\sum_{\substack{\vec{p},\vec{p}'\\ k\neq 0}} M_k^2 (C^\dagger_{\vec{p}+\vec{k}} C^\dagger_{\vec{p}'-\vec{k}} C_{\vec{p}'} C_{\vec{p}} - N) - \sum_{\vec{k},\vec{p}} M_k^2 C^\dagger_{\vec{p}+\vec{k}} C_{\vec{p}} b^\dagger(\vec{R}) b(\vec{R}) e^{-i\vec{k}\cdot\vec{R}},$$

and the electromagnetic term is

$$H_{\rm EM} = \sum_{\vec{p}} V(\vec{P}) C_{\vec{p}} b(\vec{R}) \alpha^\dagger$$

M_k^2 is the Coulomb interaction $4\pi e^2/k^2$; $C^\dagger_{\vec{p}}$ and $C_{\vec{p}}$ are, respectively, the creation and annihilation operators of the valence electron of momentum $\vec{p}$; $b^\dagger(\vec{R})$ and $b(\vec{R})$ are, respectively, the creation and annihilation operators of a core vacancy in an ion localized at $\vec{R}$; $H_{\rm EM}$ represents the x-ray emission term in which $\alpha^\dagger$ is the creation operator of an x-ray photon; and $V(\vec{P})$ is proportional to the matrix element corresponding to the transition of a valence electron of momentum $\vec{P}$ to the core vacancy. After making two appropriate canonical transformations and neglecting (i) the recoil energy of the electrons, (ii) the Doppler effect of the plasmon eigenfield of the electron, and (iii) the variation of the matrix element with the wave vector of the free electron, Brouers[5] finds the additional effective Hamiltonian as

$$H' = \left(\frac{1}{2\hbar\omega_p}\right)^{1/2} \sum_{\vec{p},\,k<k_c} M_k V(\vec{P})\, \alpha^\dagger A^\dagger_k C_{\vec{p}}\, b, \qquad (2)$$

where $A_k^\dagger$ is the creation operator of plasmon. The authors[13] have calculated the relative intensity using the above Hamiltonian H' as

$$i = \alpha\left[1 - \frac{3}{2}\left(\frac{2}{\beta}\right)^{1/2} \tanh^{-1}\left(\frac{\beta}{2}\right)^{1/2} + \frac{1}{2}\left(\frac{1}{1-\frac{1}{2}\beta}\right)\right], \qquad (3)$$

where α stands for $e^2k_c/\pi\hbar\omega_p$ which is nearly equal[14] to $\sim 0.12 r_s$, β is given by k_c/k_F, and k_c is the cut-off wave vector of the electron and separates the bosons from fermions. The above expression for the relative intensity is valid only when the electrons are taken in the bottom of the conduction band. We have calculated the relative intensities of low-energy plasmon satellites of Li, Be, and Na using Eq. (3) and the results are summarized in Table I.

It is evident from Table I that in the case of Li

TABLE I. Relative intensities of low-energy plasmon satellites of Li, Be, and Na.

Metals	r_s (Ref. 15)	α	β (Ref. 15)	Relative intensity: Authors' value	Relative intensity: Experimental value of Arakawa *et al.* (Ref. 12)
Li	3.2662	0.391 944	0.63	0.013	0.01
Be	1.8916	0.226 992	0.48	0.0039	0.008
Na	3.993	0.479 16	0.70	0.02	0.015

and Na our theoretically calculated relative intensities show remarkable agreement with the experimental values while the agreement in the case of Be is slightly poorer. Thus we can safely say that the low-energy satellites of Li, Be, and Na reported by Arakawa and Williams[7] are due to volume plasmon creation.

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