and space potential along the tube depend essentially on the gas pressure, diameter of the discharge tube and high-frequency field intensity.

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The Absorption and Emission of X-Rays in Ferromagnetic Metals

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The problem of absorption and emission of x-rays by a ferromagnetic is examined in the framework of interaction of the inner and outer electrons.

1. There has been to date no theoretical examination of the absorption and emission of x-rays by ferromagnetic substances. In view of the importance of a study of the subject, we shall attempt to solve the problem in a very rough, qualitative approximation.

In the absorption of x-rays by inner shell electrons it is essential that the frequency of the x-ray be sufficient to excite the electron into an unoccupied level above the conduction levels. By examining the fine structure of the absorption band edge, one can hope to obtain some detailed information about the highest electron energy levels in the metal.

Since the initial electron level is part of an inner shell, it can be taken as infinitely narrow. Let ψ_0 be the normalized wave function of the initial state, $\hbar\omega_{\xi' 0}$ --- the energy difference between this state and a state of conductivity k. The optical conductivity, which determines absorption, is given by the equation [1]

$$nk\nu = \sigma = -\frac{\pi e^2}{m^2\hbar\omega G^3 a^3}\sum_{ss'}\int\frac{\rho_0(\xi, s') - \rho_0(\xi, s)}{|\operatorname{grad}_\xi \omega_{\xi\xi'}|} \times |p_x(\xi, \xi')|^2\, du\, dv. \quad (1)$$

Here s is the sum index over initial states, and s' the sum index over final states of the metal electrons in the first Brillouin zone. Since, in the present case, the initial levels are essentially the discrete levels of isolated atoms, the corresponding wave function is different from zero only in a small region. This makes the summation over s easy. If there are N_0 atoms per unit volume, then we have for the optical conductivity:

[1] A. V. Sokolov, J. Exper. Theoret. Phys. USSR **25**, 9 (1953)

$$(\rho_0(\xi, s') = 0, \quad \text{and} \quad \rho_0(\xi, s) = G^3/8\pi^3)$$

$$\sigma = nk\nu = \frac{\pi e^2\hbar N_0 G^3}{8\pi^3 m^2\hbar\omega a^3}\Omega\int\{[\nabla_\xi E(\xi)]^{-1} \times |p_x(\xi, 0)|^2\}_{\omega_{\xi 0}=\omega}\, du\, dv, \quad (2)$$

where we take into account the relation

$$\omega_{\xi 0} = [E(\xi) - E(0)]/\hbar, \quad (3)$$

$E(0) = \text{const}$, is the energy of the K electron in the atom; the summation over s' in the first zone is replaced by multiplication by the number of states in unit volume of k-space.

2. With the removal of an electron from an inner shell, a conduction electron may make the transition to the vacant lower level, simultaneously emitting an x-ray quantum. Because of this, a study of the emission spectra of a metal serves as a source of information about the energy levels occupied by conduction electrons [2]. The intensity of x-rays emitted in the frequency interval ω to $\omega + d\omega$ is

$$I(\omega)\, d\omega = \frac{4N_0\omega^2\hbar^2 e^2}{3c^3 m^2} d\omega \sum_{s'}\left|\int\psi_k^*\nabla\psi_0\, d\tau\right|^2, \quad (4)$$

where the summation is carried over all occupied states of the conduction electrons with energy corresponding to a frequency ω_0 such that $\omega \leq \omega_0 \leq \omega + d\omega$, i.e., $\hbar\, d\omega = dE$.

Instead of a summation over all possible values of k, it is possible to write an integral over $(G/2\pi)^3\,\Omega_0 dk_1\, dk_2\, dk_3$; we then obtain

$$I(\omega)\, d\omega = \frac{N_0\hbar^2\omega^2 e^2 G^3\Omega_0}{6\pi^3 m^2 c^3} dE\int\left(\frac{\partial E}{\partial k_1}\right)^{-1} \quad (5)$$

[2] A. Wilson, *Quantum Theory of Metals*, pp. 42-44

$$\times \left|\int \psi_k^* \nabla \psi_0 \, d\tau\right|^2 dk_2 \, dk_3.$$

Multiplying and dividing the right side of Eq. (5) by $\hbar$, we obtain

$$I(\omega)\,d\omega = \frac{N_0\hbar^3\omega^2 e^2 G^3 \Omega_0}{6\pi^3 m^2 c^3} \frac{dE}{\hbar} \int \left(\frac{\partial E}{\partial k_1}\right)^{-1} \times \left|\int \psi_k^* \nabla \psi_0 \, d\tau\right|^2 dk_2 \, dk_3, \quad (6)$$

But $dE/\hbar = d\omega$, and, therefore, the final expression for the emitted radiation is

$$I(\omega) = \frac{N_0\hbar^3\omega^2 e^2 G^3 \Omega_0}{6\pi^3 m^2 c^3} \int \left\{\left(\frac{\partial E}{\partial k_1}\right)^{-1} \times \left|\int \psi_k^* \nabla \psi_0 \, d\tau\right|^2\right\}_{\omega_{k0}=\omega} dk_2 \, dk_3. \quad (7)$$

Examining Eqs. (2) and (7), we see that both absorption and emission of x-rays is determined by the quantity

$$F = F_1 + F_2 + F_3 = \int \left\{\left(\frac{\partial E}{\partial k_1}\right)^{-1} \times \left|\int \psi_k^* \nabla \psi_0 d\tau\right|^2\right\} dk_2 \, dk_3. \quad (8)$$

This quantity is determined both by the density of conduction electron states, and by the transition probability.

3. For the generalization of the calculation of absorption and emission of x-rays by ferromagnetic metals, using band theory, we shall use a model (originally proposed by Vonsovskii) of exchange interaction between outer s and inner d electrons. In the following we shall use the same notation as in the calculation of conduction electron state density in a ferromagnetic, that is κ_1 --- the component of the wave vector perpendicular to the boundary plane, and κ_2 and κ_3 --- components parallel to this plane.

For the wave function of the s electron we shall use a Brillouin function. All the coefficients of a Fourier expansion of the potential are real and negative for a simple lattice; then for small values of κ_1 the unnormalized wave function for conduction electrons has the form:

$$\psi_k^{(B)} = e^{i\vec{\kappa}\mathbf{r}} \sin \pi |\mathbf{g}| x \quad \text{(upper band)}$$

$$\psi_k^{(H)} = e^{i\vec{\kappa}\mathbf{r}} \cos \pi |\mathbf{g}| x \quad \text{(lower band)}$$

If the x-ray level is in the K-shell, then ψ_0 has spherical symmetry, and the corresponding transition probability is determined by the expression

$$\int \psi_0^* \frac{\partial \psi_k^{(B)}}{\partial x} d\tau = \int \exp[-\lambda r + i\vec{\kappa}\mathbf{r}] \times (i\kappa_1 \sin \pi |\mathbf{g}| x + \pi |\mathbf{g}| \cos \pi |\mathbf{g}| x)\, d\tau = M, \quad (9)$$

$$\int \psi_0^* \frac{\partial \psi_k^{(H)}}{\partial x} d\tau = \int \exp[-\lambda r + i\vec{\kappa}\mathbf{r}] \times (i\kappa_1 \cos \pi |\mathbf{g}| x - \pi |\mathbf{g}| \times \sin \pi |\mathbf{g}| x)\, d\tau = \kappa_1 M',$$

where M and M' are quantities independent of κ_1 in the first approximation; λ for the K-shell is approximately Z/a_0 --- the atomic number divided by the radius of the first atomic orbit.

We shall carry out the calculation as in reference 5. Calculation of F for a state in the lower band proceeds as follows in ordinary band theory. We use Eq. (8), and need to find the density of states and the transition probability. The first is

$$\left(\frac{\partial E}{\partial \kappa_1}\right)^{-1} = \frac{m}{\pi\hbar^2 g} \frac{\Gamma}{(\Gamma^2 - |V_g|^2)^{1/2}},$$

The second, using Eq. (10), is

$$\left|\int \psi_k^* \nabla_x \psi_0 \, d\tau\right|^2 = \kappa_1^2 M'^2.$$

Taking into account that

$$\kappa_1^2 = \frac{m^2}{\pi^2\hbar^4 g^2}(\Gamma^2 - |V_g|^2) \quad \text{and that}$$

$$d\kappa_2 \, d\kappa_3 = -\frac{m}{\hbar^2} d\Gamma \, d\varphi,$$

we have

$$F_1 = \int \frac{m}{\pi\hbar^2 g} \frac{\Gamma}{(\Gamma^2 - |V_g|^2)^{1/2}} \kappa_1^2 M'^2 \frac{m}{\hbar^2} d\Gamma \, d\varphi = \frac{2m^4 M'^2}{\pi^2\hbar^8 g^3} \int \sqrt{\Gamma^2 - |V_g|^2}\, \Gamma \, d\Gamma. \quad (11)$$

To obtain the analogous quantity in the case of a ferromagnetic metal, we consider the electrons as a mixture of two gasses with respective spins s^+ and s^-. In this case we can write

$$m_\pm = m_1 / (1 \pm (\beta'/\beta) y); \quad (12)$$

$$\sqrt{\Gamma_\pm^2 - |V_g|^2} = (1 \pm (\beta'/\beta) y) \sqrt{\Gamma^2 - |V_g|^2},$$

$$\Gamma_\pm \, d\Gamma'_\pm = (1 \pm (\beta'/\beta) y)^2 \, \Gamma \, d\Gamma.$$

Substituting Eq. (12) into Eq. (11), we obtain

$$F_1^\pm = \frac{2m_1^4 M'^2}{\pi^2\hbar^8 g^3} \frac{1}{(1 \pm (\beta'/\beta) y)} \int \sqrt{\Gamma^2 - |V_g|^2}\, \Gamma \, d\Gamma. \quad (13)$$

Adding F_1^+ and F_1^-, we obtain

$$F_1(E,\gamma)=\frac{4m_1^4M'^2}{\pi^2\hbar^8 g^3}(1+A^2\gamma^2)\int\sqrt{\Gamma^2-|V_g|^2}\,\Gamma\,d\Gamma \tag{14}$$

Carrying out a similar calculation for the upper band, we have

$$F_1(E,\gamma)=\frac{4m_1^2M^2}{\hbar^4 g}(1+A^2\gamma^2)\int\frac{\Gamma\,d\Gamma}{\sqrt{\Gamma^2-|V_g|^2}} \tag{15}$$

The changes of F are therefore determined by the following three quantities:

I) $E<V_{000}+E_g-|V_g|$: (16)

$$F_1(E,\gamma)\sim\frac{4}{3}\frac{m_1^4M'^2}{\pi^2\hbar^8 g^3}(1+A^2\gamma^2)\left[(E_g^2-|V_g|^2)^{3/2}-\{(V_{000}+E_g-E)^2-|V_g|^2\}^{3/2}\right];$$

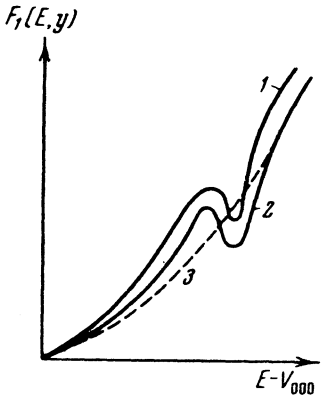
II) $V_{000}+E_g-|V_g|<E<V_{000}+E_g+|V_g|$: (17)

$$F_1(E,\gamma)\sim\frac{4}{3}\frac{m_1^4M'^2}{\pi^2\hbar^8 g^3}(1+A^2\gamma^2)(E_g^2-|V_g|^2)^{3/2};$$

III) $V_{000}+E_g+V_g<E$; (18)

$$F_1(E,\gamma)\sim\frac{4}{3}\frac{m_1^4M'^2}{\pi^2\hbar^8 g^3}(1+A^2\gamma^2)(E_g^2-|V_g|^2)^{3/2}+\frac{4m_1^2M^2}{\hbar^4 g}(1+A^2\gamma^2)\{(E-E_g-V_{000})^2-|V_g|^2\}^{1/2}$$

In this calculation we have taken into account only the **g** and **– g** planes. Therefore the deviation of of the $F_1(E,\gamma)$ curve from the corresponding curve for free electrons must be multiplied by the number of pairs of equivalent planes which bound the first zone. The quantities $F_2(E,\gamma)$ and $F_3(E,\gamma)$, corresponding to radiation with electric vector parallel to the discontinuity (boundary) plane, can also be easily calculated. It turns out that they have the same general form as $F_1(E,\gamma)$, with the exception that their derivatives are everywhere continuous. Thus the form of $F(E,\gamma)$ is primarily determined by $F_1(E,\gamma)$ (see Figure).



K radiation
1 --- $F_1(E,\gamma)$
2 --- $F_1(E,0)$
3 --- free electrons

The curve $F_1(E,\gamma)$ for *K* radiation is somewhat higher than $F_1(E,0)$ in the absence of magnetization. To observe this effect one should examine the emission spectra of ferromagnetic metals (which are experimentally convenient) above and below the ferromagnetic Curie point. From Eqs. (14) and (15) it follows that the difference of ordinates of the $F_1(E,\gamma)$ and $F_1(E,0)$ curves can be several percent of the value for the unmagnetized state.

4. Thus, in the framework of an *s* -- *d* exchange model it is shown that the emission and absorption of x-rays by ferromagnetic metals must depend on the spontaneous magnetization. In the vicinity of the ferromagnetic Curie point this dependence is quadratic [Eqs. (14) - (18)].

Additional Footnotes:

[3] S. V. Vonsovskii, J. Exper. Theoret. Phys. USSR **16**, 981 (1946)

[4] S. V. Vonsovskii and E. A. Turov, J. Exper. Theoret. Phys. USSR **24**, 419 (1953)

[5] A. V. Sokolov and S. M. Tsipis, J. Exper. Theoret. Phys. USSR **28**, 321 (1955); Sov. Phys. **1**, 218 (1955)

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