THEORY OF SPECTRAL COMPOSITION OF PHOTO-EMITTED ELECTRON FLUXES

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Analytical expressions are obtained for the relationship between the initial nonequilibrium energy distribution of optically excited electrons within a material and the spectral composition of the flux of electrons emitted into a vacuum. The change in the character of photoelectron transport in the emission active layer caused by electron–phonon interaction and the redistribution over energy produced by such interaction are considered.

Upon continuous irradiation of a semiconductor by light there develops within its volume a steady-state nonequilibrium excited electron distribution. The fraction of electrons with energies exceeding the vacuum level may reach the surface and be emitted into the vacuum. During transport the excited nonequilibrium electrons undergo scattering on lattice oscillations, structural defects, boundaries of the emission-active layer of the material, and can also scatter with formation of electron–hole pairs. Information on these processes and the energetic electron structure of the crystal can be obtained by analysis of the observed photoelectron emission spectra. Therefore it is of importance to establish the interrelationship between the original nonequilibrium distribution of optically excited electrons within the material and the energy distribution of the electrons exiting the crystal.

Among the various factors responsible for the spectral composition of the emitted electron flux, an important role is played by the processes of scattering of photo-excited electrons on phonons. Upon emission or absorption of a phonon, there occurs a redistribution of electrons over energy, so that after n acts of e–p scattering the distribution differs from the original one $N_0(E)$ and generally speaking, is defined by another function, $N_n(E)$.

Moreover, the directions of propagation of photo-excited electrons are chaotized in electron–phonon interactions, which changes their transport conditions in principle, and thus, significantly changes the probability of reaching the emitting surface.

Electron transport is also controlled by the action of other scattering mechanisms. Thus, for electrons with energies exceeding the amount required for formation of electron–hole pairs, an inelastic scattering (e–e scattering) channel is opened. One must also note the important role in forming the structure of the spectrum of photo-emitted electrons of electron-scattering processes involving the surface.

These mechanisms produce varied, sometimes competing, effects, so that their combined action leads to a complex and ambiguous picture. Therefore a proper interpretation of experimental results must be based on a theory which considers the effects of such interactions in detail.

Let the probability $p_\omega(x)$ characterize the spatial distribution of electrons excited in the volume of the emission-active layer due to intrinsic optical absorption, while $p_n(x; E)$ is the probability of exit of an electron from depth x into the vacuum after n acts of e–p scattering (with consideration of attenuation caused by the presence of an inelastic scattering channel). Then the energy distribution function for the emitted electrons can be represented in the following form:

$$N(E,\ \omega) = \sum_{n=0}^{\infty} N_n(E) \int_0^h p_\omega(x) p_n(x;\ E)\, dx, \qquad (1)$$

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where h is the layer thickness, ω is the frequency of the exciting light, E is the electron energy. In writing Eq. (1) only those electrons exiting into the vacuum were considered which did not excite secondary excitations during the transport process.

We will introduce the following notation: let u and v be the probabilities of emission and absorption of a phonon by an electron in the e–p interaction, while $\bar{E}_p$ is the mean phonon energy

$$P_n = \int_0^h p_\omega(x)\, p_n(x;\, E)\, dx.$$

For the function $N_n(E)$ we can write the recursive relationship

$$N_n(E) = uN_{n-1}(E+\bar{E}_p) + vN_{n-1}(E-\bar{E}_p), \tag{2}$$

which allows reduction of Eq. (1) to the following form:

$$N(E,\,\omega) = N_0(E)\, A_0 + \sum_{n=1}^{\infty}\left[\left(\frac{u}{v}\right)^{n/2} N_0(E+n\bar{E}_p) + \left(\frac{v}{u}\right)^{n/2} N_0(E-n\bar{E}_p)\right] A_n, \tag{3}$$

$$A_n = \sum_{\kappa=0}^{\infty} P_{n+2\kappa}\frac{(n+2\kappa)!}{\kappa!\,(n+\kappa)!}(uv)^{\kappa+\frac{n}{2}}. \tag{4}$$

We will manipulate the last equation. We introduce the total probability of electron exit into the vacuum: $G = \sum_{n=0}^{\infty} P_n$. This quantity can be considered as a function of the parameter $\beta = \ell/\ell_p$ and written in the form of an expansion in a series in powers of β ($\ell^{-1} = \ell_p^{-1} + \ell_e^{-1}$; ℓ_p and ℓ_e being the mean electron path lengths between e–p and e–e scattering acts respectively). It follows from the definitions of the probabilities $G(\beta)$ and P_n that

$$P_n = \frac{\beta^n}{n!}\left[\frac{\partial^n}{\partial\beta^n} G(\beta)\right]_{\beta=0}. \tag{5}$$

Considering the well-known [1] expansion of the modified Bessel function

$$I_n(z) = \sum_{\kappa=0}^{\infty}\frac{(z/2)^{2\kappa+n}}{\kappa!\,(n+\kappa)!}, \tag{6}$$

we write Eq. (4) in the form

$$A_n = \hat{I}_n\left(2\beta\sqrt{uv}\,\frac{\partial}{\partial\beta_1}\right) G(\beta_1)\,|_{\beta_1=0}, \tag{7}$$

where $\hat{I}_n$ is a modified Bessel function of the operator.

Substituting Eq. (7) in Eq. (3) and considering that $I_n(z)$ is an even function, for $N(E, \omega)$ we obtain the expression

$$N(E,\,\omega) = \sum_{n=-\infty}^{\infty}\left(\frac{u}{v}\right)^{n/2} N_0(E+n\bar{E}_p)\,\hat{I}_n\left(2\beta\sqrt{uv}\,\frac{\partial}{\partial\beta_1}\right) G(\beta_1)\,|_{\beta_1=0}, \tag{8}$$

which can easily be reduced to a form convenient for calculations. To do this we must clarify the action of the operator $\hat{I}_n$ on the function $G(\beta)$. For this purpose we may use one of the integral representations of the modified Bessel function $I_n(z)$.

We may consider, for example, the form

$$I_n(z) = \frac{1}{\pi}\int_0^{\pi} e^{z\cos\theta}\cos(n\theta)\, d\theta. \tag{9}$$

The operator $\exp\left(a\frac{\partial}{\partial\beta}\right)$ is a shift operator in the argument β, such that

$$\hat{I}_n\left(2\beta\sqrt{uv}\,\frac{\partial}{\partial\beta_1}\right) G(\beta_1)\,|_{\beta_1=0} = \frac{1}{\pi}\int_0^{\pi}\cos(n\theta)\, G(2\beta\sqrt{uv}\cos\theta)\, d\theta. \tag{10}$$

Equations (8), (10) contain the distribution function $N_0(E)$ and the total probability of electron exit into the vacuum G. The function $N_0(E)$ is defined by the structure of the electron energy spectrum of the material and the mechanisms of optical electron excitation in concrete crystals, so that it may be regarded as initial data. There exist quite well-developed methods [2-4] which allow numerical calculations of the function $N_0(E)$. The problem of calculating the total probability G with consideration of the photo-electron scattering mechanisms treated in the present study has also been studied well. Analytical expressions for this probability have been obtained for various systems: a) semi-infinite medium with one- [5], two- [6], and three-dimensional [7, 8] electron propagation patterns; b) emission-active layer of finite thickness in the one-dimensional model [9].

Thus, we have expressed the energy distribution function $N(E, \omega)$ in terms of known quantities.

The expressions thus obtained, Eqs. (8) and (10), are quite general in character and can be used for calculations of the spectral composition of the emitted electron flux. In their derivation no assumptions were made relative to the structure of the initial electron energy distribution $N_0(E)$, the character of attenuation of the exciting light within the material, or the geometry of the emitter. We will also note that calculation of $N(E, \omega)$ does not require knowledge of the intermediate distributions $N_n(E)$ or the individual probabilities P_n.

We will now turn to a simple model of the energy distribution of the optically excited electrons. We will assume that $N_0(E)$ is a Lorentz distribution with half-width γ. (Generalization to the case of a superposition of such distributions is fully obvious.) It will then be convenient to use the representation:

$$N_0(E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp\left[-\gamma|t| + i(E - E_0)t\right] dt. \qquad (11)$$

Substituting Eq. (11) in Eq. (8) and summing with the aid of the function

$$\exp\left[\frac{z}{2}\left(t + \frac{1}{t}\right)\right] = \sum_{n=-\infty}^{\infty} t^n I_n(z), \qquad (12)$$

we arrive at the expression

$$N(E, \omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt e^{-\gamma|t| + i(E-E_0)t} \exp\left[\beta\left(ue^{i\bar{E}_p t} + ve^{-i\bar{E}_p t}\right)\frac{\partial}{\partial\beta_1}\right] G(\beta_1)|_{\beta_1=0}. \qquad (13)$$

Here we again meet with action of the shift operator, so that

$$N(E, \omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\gamma|t| + i(E-E_0)t} G\left(\beta\left(ue^{i\bar{E}_p t} + ve^{-i\bar{E}_p t}\right)\right) dt. \qquad (14)$$

The function G in Eq. (14) is an analytic extension of the total probability function into the complex region for the parameter β.

Further transformation of the last expression leads to the form:

$$N(E, \omega) = \frac{1}{\pi\bar{E}} \operatorname{Re}\left\{(1 - e^{-2\pi\tilde{\gamma} + 2\pi i\tilde{E}})^{-1} \int_0^{2\pi} e^{-\tilde{\gamma}t + i\tilde{E}t} G(\beta(\cos t + i(u - v)\sin t)) dt\right\}. \qquad (15)$$

In writing Eq. (15) the notation $\tilde{\gamma} = \gamma/\bar{E}_p$, $\tilde{E} = (E - E_0)/\bar{E}_p$ was used, and it was considered that $u + v = 1$.

The integrand of Eq. (15) contains an exponentially decreasing factor $\exp(-\tilde{\gamma}t)$. Therefore for large values of $\tilde{\gamma}$ the attenuation interval is so small that the major contribution to the integral is produced by small values of t. If the change in the function G is also small, then Eq. (15) takes on the form

$$N(E, \omega) = \frac{1}{\pi}\frac{\gamma}{\gamma^2 + (E - E_0)^2} G(\beta) = N_0(E) G(\beta). \qquad (16)$$

This means that in the case considered the effect of electron redistribution over energy in e–p interactions does not play a significant role in formation of photo-emission spectra. However it must be noted that the assumption made in deriving Eq. (16) of smallness of the change in G in Eq. (15) has a limited range of applicability. Thus, it is undoubtedly invalid if the energy of the photo-ionized electrons lies below the electron–hole pair formation threshold: for such energies the complex function G in the vicinity of the point t = 0 is intensely dependent on t.

In conclusion, we will consider the basic features of the evolution of the electron energy distribution within the material upon transition from the distribution $N_0(E)$ in the form of Eq. (11) to $N_n(E)$.

Multiple application of Eq. (2) yields the expression

$$N_n(E)=\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\gamma|t|+i(E-E_0)t}\,(ue^{i\bar{E}_p t}+ve^{-i\bar{E}_p t})^n\,dt, \qquad (17)$$

which can conveniently be written in the form

$$N_n(E)=\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\gamma|t|+i(E-E_0)t}\,\rho^n(t)\,e^{in\varphi}\,dt, \qquad (18)$$

where $\rho = \sqrt{\cos^2(E_p t)+(u-v)^2\sin^2(\bar{E}_p t)}$, $\varphi = \tan^{-1}[(u-v)\tan(\bar{E}_p t)]$.

It is obvious that in the region of small t the phase φ behaves as $\varphi = (u-v)\bar{E}_p t$. But it is just this region which produces the main contribution to the integral of Eq. (18) because of rapid attenuation of the integrand; the factors $\exp(-\gamma|t|)$ and ρ^n (for large n) may act as attenuation factors. These facts permit the conclusion that the center of the distribution $N_n(E)$ shifts toward lower energies by an amount $n(u-v)\bar{E}_p$. The physical interpretation of this result is completely obvious, for the quantity $(u-v)\bar{E}_p$ has the sense of the mean electron energy loss in one act of e–p scattering.

It follows from Eq. (18) that for large values of the broadening parameter γ the form of the distribution $N_n(E)$ distorts only slightly with growth in n. The situation is entirely different for small γ values: with increase in n the attenuation interval for the function $\rho^n(t)$ decreases and becomes small in comparison to γ^{-1}, which is qualitatively equivalent to intense broadening of the distribution $N_n(E)$.

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