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Contribution of light holes to thermionic field emission in Si and Ge

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Light holes (LH) may give the main contribution to the thermionic field-emission (TFE) current through grain boundaries in Si and Ge. In spite of only a small concentration, the LH dominate because their transmission probability through the potential barrier may be several orders of magnitude larger than the probability for the heavy holes (HH). In order to explain the temperature dependence of the TFE current, previous authors were forced to introduce a lowering of the potential barrier with decreasing temperature. However, taking into account the contribution of the LH in TFE is equivalent to a lowering of the potential barrier because it results in a slower decrease of the current than found in previous calculations with only one type of holes.

Polycrystalline semiconductor films are studied intensively because they are one of the important elements of microelectronics and they are widely used for solar energy conversion instead of noneconomical single-crystalline materials.[1] Polycrystalline *p*-Si conducting leads show a large temperature coefficient of resistivity which is caused by the strong temperature dependence of the resistance of grain boundaries.[2–4] This dependence has been explained within the framework of the thermionic emission (TE),[3] and thermionic field emission (TFE).[4] As far as TFE is concerned, the conventional theory is based[5,6] on a one-dimensional time-independent WKB transmission probability τ for potential barrier:[7]

$$\tau(E)=\exp\left(-2\int_{x_1}^{x_2}\{2m^*[qV(x)-E]\}^{1/2}dx\Big/\hbar\right) . \quad (1)$$

Here, x_1 and x_2 are the classical turning points of the carriers with an energy E associated with the component of momentum in the x direction normal to the interface, $qV(x)$ the charge-carrier potential energy in the depletion region caused by the grain boundary, and m^* the effective mass of the charge carrier.

In *p*-Si and *p*-Ge there are two different types of holes: light holes (LH) and heavy holes (HH) with different effective masses $m_L^*=m_1m_0$ and $m_H^*=m_2m_0$, where m_0 is the free-electron mass (in Si: $m_1=0.16$, $m_2=0.52$; in Ge: $m_1=0.043$, $m_2=0.34$, Ref. 8). Most treatments, however, have thus far used only one equivalent carrier effective mass $m^*=mm_0$ (for Si, e.g., in Ref. 4 $m=0.386$). Since $m_1 \ll m_2$, the transition probability τ for the LH may easily be larger than for that of the HH by several orders of magnitude. In these cases the current through the grain boundary calculated by the approach developed here differs by an appreciable amount from previous works where equivalent carrier effective mass were used. It is the purpose of the present paper to consider the two carrier types in detail and to calculate their relative contributions to thermionic transport.

Let us consider in Fig. 1 the same potential-energy diagram for an individual grain boundary in a *p*-type semiconductor as done earlier by Lu and co-workers.[4] The space-charge potential barrier has the height V_B and width W. The usual relation between V_B, W, and doping concentration N in the grain is satisfied: $W^2=2\epsilon V_B/(qN)$, where ϵ is the static permittivity. An additional rectangular barrier with a width δ and height H, is assumed. This energy diagram with additional barrier, where both width δ and height H are allowed to vary with temperature in order to achieve a force fit to experimental data,[4] is physically questionable. This potential-energy diagram is used here only to demonstrate the importance of contribution of the LH in the TFE through rectangular barrier ($V_B=0$ on Fig. 1) and through space-charge potential barrier ($\delta=0$), as well as in the common case, which was analyzed by Lu and co-workers.[4]

For small applied voltages U, satisfying $qU/kT \ll 1$, it is easy to obtain the net current density J of two types of carriers by using a method similar to the one used[3–6] for only one type.

$$J=BI,\quad B=q^2p\frac{U}{\sqrt{2\pi kT}}\frac{m_L^*+m_H^*}{m_L^{*3/2}+m_H^{*3/2}} , \quad (2)$$

$$I=\sum_{i=1}^{2}\frac{m_i}{m_1+m_2}\int_0^\infty\frac{dE}{kT}\exp\left(\frac{E}{kT}-C_i(E)\right) , \quad (3)$$

$$C_i(E)=2\sqrt{m_i}\frac{\sqrt{2m_0}}{\hbar}\left[\eta(E_B-E)\left\{\left(1-\frac{E}{E_B}\right)^{1/2}+\frac{E}{E_B}\ln\left\{\left[1-\left(1-\frac{E}{E_B}\right)^{1/2}\right]\Big/\left(\frac{E}{E_B}\right)^{1/2}\right\}\right\}W\sqrt{E_B}+\eta(H-E)\left(1-\frac{E}{H}\right)^{1/2}\delta\sqrt{H}\right], \quad (4)$$

$$\eta(X)=\begin{cases}1 \text{ for } X>0\\ 0 \text{ for } X<0.\end{cases}$$

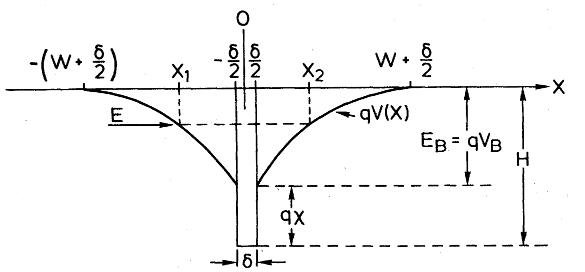

FIG. 1. Potential-energy diagram of a grain boundary in p-Si.

Here, p is hole concentration in homogeneously doped crystalline and U the voltage applied across the potential barrier; U is assumed to be equally divided on each side of the symmetrical semiconductor to semiconductor junction.[3,4,9]

The coefficients $C_i(E)$ are obtained by integration of Eq. (1). The first term in $C_i(E)$ is responsible for TFE through a space-charge barrier of height E_B and width W at the basis and the second term for TFE through a rectangular barrier of height H and width δ (see Fig. 1).

For $E > H$, we have $C_i \equiv 0$. Equation (3) can be integrated from H to ∞ and one can obtain the usual expression for TE

$$I_{\mathrm{TE}} = \exp(-H/kT) \ , \tag{5}$$

where H is the barrier height. If the tunneling probability is small [i.e., $C_i(E)$ is large] the integral from 0 to H in (3) gives only a small contribution to I in comparison with I_{TE}. In this case $I \cong I_{\mathrm{TE}}$, and the net current J is determined by TE. The integrals (3) for the LH and the HH are equal, except that the prefactors of the first one are smaller, being $m_1(m_1+m_2)$, than before the second integral, which is $m_2/(m_1+m_2)$. To get I_{TE} in the conventional form (5), we have included $m_L^* + m_H^*$ in the coefficient B (2).

The following points are important.

(1) The contribution of the LH to the current J amounts to a (m_1/m_2) share of the contribution of the HH and is larger than the contribution of the LH to the density of states which is proportional to $(m_1/m_2)^{3/2}$.

(2) The appropriate transport effective mass m_t^*, which determines the current in Eq. (2), is

$$1/m_t^* = [(m_L^* + m_H^*)/(m_L^{*(3/2)} + m_H^{*(3/2)})]^2 \tag{6}$$

and equals neither the effective mass m_D^* of the density of states $m_D^* = (m_L^{(3/2)} + m_H^{*(3/2)})^{2/3}$, nor the effective mass m_c^* of the conductivity, which is introduced for equal scattering times LH and HH as[10]

$$m_c^* = (m_L^{*(3/2)} + m_H^{*(3/2)})/m_L^{*(1/2)} + m_H^{*(1/2)}) \ .$$

Previously[3,4] m_c^* was used in TF and TFE calculations as an equivalent carrier effective mass. For TE currents, it gave no essential difference compared with the exact results (2) because $m_t^*/m_c = 1.06$ in Si and 1.116 in Ge.

Next, let us analyze the contribution of TFE to the net current, in the case $W^2 E_B \ll \delta^2 H$, when only the rectangular barrier matters and only the second term is preserved in $C_i(E)$ in Eq. (4). In the energy range $E < H$ the sign of the first derivative with respect to the energy of the integrand of Eq. (3) equals the sign of the expression

$$D_i(E) = -[1 - \sqrt{2m_i m_0/(H-E)}\delta kT/\hbar] \ . \tag{7}$$

For $E \to H$ we have $D_i > 0$ and $D_i > 0$ for all energies E, if

$$F_i \equiv \sqrt{2m_i m_0/H}\,\delta kT/\hbar > 1 \ . \tag{8}$$

Barriers for which $F_i \gg 1$ are defined as "wide." To estimate F_i from Eq. (8), one can use the following units: kT and H in eV, δ in Å, and taking $\sqrt{2m_0}/\hbar = 0.5012$ as a dimensionless constant. At room temperature the barrier with $H = 0.2$ eV is "wide" for the heavy holes in Si if $\delta > 47$ Å and for the light holes in Si if $\delta > 85$ Å. The TFE current through a "wide" barrier is determined by the electrons tunneling near the top of the barrier. The integral of Eq. (3) can be solved analytically:

$$I = I_{\mathrm{TE}} + I_{\mathrm{TFE}}, \quad I_{\mathrm{TFE}} = \frac{1}{m_1+m_2}\frac{\hbar^2}{2m_0\delta^2 kT}\exp(-H/kT) \ . \tag{9}$$

The contributions of the LH and the HH to the I_{TFE} in Eq. (9) are exactly identical. The small coefficient m_1 in front of the integral of Eq. (3) for the LH is compensated by the larger value of the integral compared with that for the HH. If $H \lesssim kT$, barrier was no importance. But, if $H \gg kT$, I_{TFE} [see Eq. (9)] for the "wide" barrier is small in comparison with $I_{\mathrm{TE}}(5)$. The contribution of I_{TFE} to I increases when T decreases.

When the temperature decreases, the inequality (8) breaks down before I_{TFE} dominates over I_{TE}, and it is interesting to consider the case $F_i \ll 1$. Such barriers are defined as "narrow," and $D_i(E)$ of Eq. (7) changes sign, when E increases from 0 to H. It means that the integrand of Eq. (3) has a maximum at an energy E small in comparison with H. The integration of Eq. (3) then results in

$$I_{\mathrm{TFE}} = \sum_{i=1}^{2}\frac{m_i}{m_1+m_2}\exp\left(-2\sqrt{m_i}\frac{\sqrt{2m_0H}\,\delta}{\hbar}\right)\frac{1-\exp[-(H/kT)(1-F_i)]}{1-F_i} \ . \tag{10}$$

Since $F_i \ll 1$ and $H \gg kT$, the last fraction is close to one. The contribution of the LH to I_{TFE} exceeds that of the HH whenever

$$2\sqrt{2m_0H}\,\delta(\sqrt{m_2}-\sqrt{m_1})/\hbar \equiv 2H(F_2-F_1)/kT > \ln(m_2/m_1) \ . \tag{11}$$

For the "narrow" barrier it is $I_{\mathrm{TFE}} \gg I_{\mathrm{TE}}$ [compare (10) and (5)]. If the inequality (11) holds, the total current J is determined by TFE of the LH. This current of the LH will also be larger than the current calculated in a one-band approximation if the inequality

$$2\sqrt{2m_0H}\,\delta(\sqrt{m_2}\{[1+(m_1/m_2)^{3/2}]/[1+(m_1/m_2)^{1/2}]\}^{1/2}-\sqrt{m_1})/\hbar > \ln(\{[1+(m_1/m_2)^{3/2}][1+(m_1/m_2)^{1/2}]\}^{1/2}m_2/m_1) \tag{12}$$

holds. Inequalities (11) and (12) differ only by unessential square roots of the order of unity. This means that if the main contribution to the current is determined by LH, then this current is larger than the current calculated in a one-band approximation in previous publications.

The usual expression for one type of carrier is not at all applicable, if LH mainly contribute to I_{TFE}. In the exponent of Eq. (10) one has the LH effective mass, but in the preexponential factor, as it is possible to see from Eqs. (10) and (2) it is $1/(m^*)^{1/2}$, where the effective mass $m^* = m_H^*(m_H^*/m_L^*)^2 >> m_H^*$.

When the temperature T decreases, the transition from a "wide" ($F_l > 1$) to "narrow" barrier ($F_l < 1$) takes place. An increased contribution of the LH to the current results.

If $\delta^2 H << W^2 E_B$ and only the space-charge barrier matters, the I_{TFE} for the "narrow" barrier will differ from Eq. (10) only by the insignificant last fraction if one substitutes δ and H by W and E_B, respectively. For the "wide" barrier, the contribution of the LH to the I_{TFE} will be $(m_1/m_2)^{2/3}$ of the contribution of the HH.

To demonstrate the influence of the LH on the net current J we show in Fig. 2 the dependence of I on δ for three different values of χ (see Fig. 1) for the case $N = 8.92 \times 10^{17}$ cm^{-3}, $E_B = 0.078$ eV, which was analyzed in detail in Ref. 4. The result of Ref. 4 for a one-band approximation with equivalent effective mass $m^* \equiv m_c^* = 0.386 m_0$ is shown by the dashed curves, while the present calculations (2)–(4) are given by solid curves.

At room temperature and $\chi = 0.1$ V the difference in the two calculations is small because, for $\delta \equiv 0$, the influence of the rectangular barrier vanishes and I is close to $I_{TF}(\delta = 0)$. From Eq. (5) with $H = E_B$ we have that $\log_{10} I_{TE}(\delta = 0) = -1.31$ for $T = 298$ K and -2.65 for $T = 148$ K. (These values are shown as crosses on the ordinate of Fig. 2.) For large δ again I is close to $I_{TE}(H)$, which is determined from (5) with $H = E_B + q\chi$. On the Fig. 2 $I_{TE}(H)$ is shown by dot-dashed curves.

When χ increases, $I_{TE}(H)$ decreases and the contribution of I_{TFE} to I increases. The difference between the two calculations becomes then considerable. For $T = 148$ K the discrepancy is large even for $\chi = 0.1$ V. It reaches two orders of magnitude for $\chi = 0.5$ V.

This comparison demonstrates the necessity of taking into account both types of holes in p-Si for the modeling and optimization of polycrystalline silicon resistors.[3]

We conclude this paper with a short summary of principal results. The contribution of the LH to the TFE current increases, when the temperature T decreases. This contribution becomes larger than the contribution of the HH, when the current itself becomes sufficiently larger than the current calculated for the given barrier with the only TE taken into account. This result does not depend on the form and on the parameters of the potential barrier.

For the p-Ge the role of the LH and the difference between the calculations with the real m_L^* and m_H^* and with the equivalent carrier effective mass $m^* = m_c^*$ is considerable because the ratio m_2/m_1 for Ge is greater than for Si.

The approach described here may be used for the TFE from the grain boundary interface states[11] of p-Si and p-Ge.

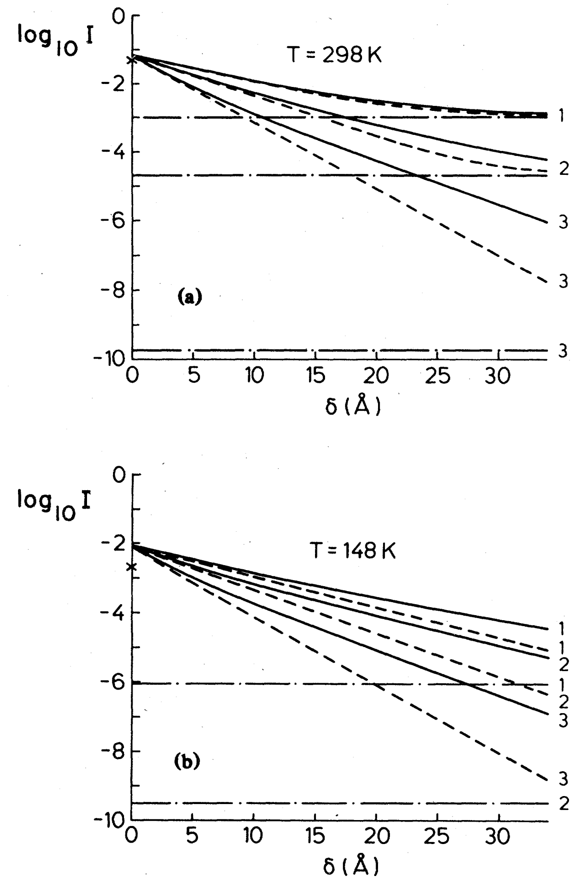

FIG. 2. Dependence of $\log_{10} I$ on rectangular barrier width δ for $T = 298$ K (a), and $T = 148$ K (b) for different additional rectangular barrier heights $\chi = 0.1$ V(1), 0.2 V(2), and 0.5 V(3). Solid curves show present calculation with masses $m_1 = 0.16$ and $m_2 = 0.52$; dashed curves show the results of Lu *et al.*[4] for the one-band approximation with mass $m^* = 0.38$; and dash-dotted curves show the $\log_{10} I_{TE}$ from Eq. (5) for $H = E_B + q\chi$.

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