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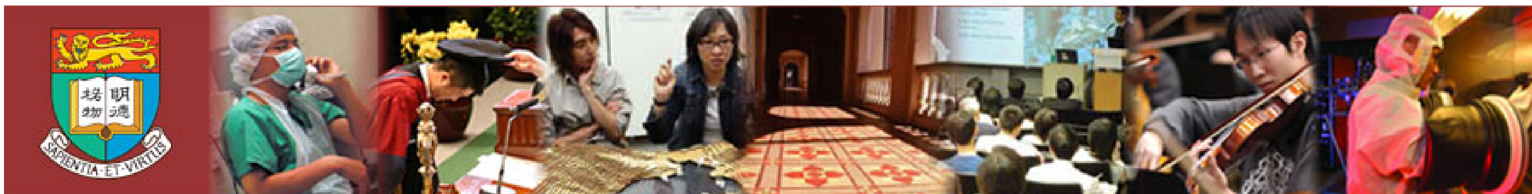

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Numerical modeling of transient characteristics of photovoltage in Schottky contacts

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Numerical modeling of the transient characteristics of the photovoltage at metal-semiconductor interfaces has been carried out with a simple model in which the contributions of different current transport processes including thermionic emission, tunneling, carrier recombination, and leakage current have been taken into account. The simulation gives the detailed dependence of the transient characteristics on temperature, doping concentration, Schottky barrier height, and leakage resistance. © *1994 American Institute of Physics.*

Under illumination of a Schottky contact, electron-hole pairs are generated in the depletion region by photon excitation, and these electron-hole pairs will then be separated by the built-in field of the Schottky barrier. The generation and the separation of the electron-hole pairs produce a photocurrent J_{pc} within the depletion region. At the same time, a photovoltage V across the depletion region is also established. Obviously, the thermal-equilibrium condition of the metal-semiconductor system is disturbed by the illumination. Processes exist to restore the system to equilibrium. These processes may include thermionic emission over the barrier, tunneling through the barrier, recombination in the depletion region, and leakage current. Therefore, the photocurrent is countered by a restoring current J due to these processes.

The charge change dQ/dt in the depletion region can be written as

$$J_{pc}-J=\frac{dQ}{dt}. \tag{1}$$

dQ can also be expressed as

$$dQ=C\,dV, \tag{2}$$

where C is the capacitance per unit area of the depletion region, given by[1]

$$C=\left(\frac{q\epsilon_s N_d}{2(\Phi_b-V-V_n)}\right)^{1/2}, \tag{3}$$

where ϵ_s is the dielectric constant of the semiconductor, N_d is the semiconductor's doping concentration, $q\Phi_b$ is the Schottky barrier height, and qV_n is the energy difference between the conduction-band minimum and the Fermi level in the bulk of the semiconductor.[1] According to Eqs. (1)–(3) and assuming that the photovoltage is $V_1(t_1)$ and $V_2(t_2)$ at time t_1 and t_2, respectively, we obtain the following relation:

$$t_2-t_1=\int_{V_1(t_1)}^{V_2(t_2)}\left(\frac{q\epsilon_s N_d}{2(\Phi_b-V-V_n)}\right)^{1/2}\frac{1}{J_{pc}(t)-J(V)}\,dV. \tag{4}$$

For simplicity, we assume that the variation of J_{pc} with t is a square wave. The initial condition for Eq. (4) can be defined as $V(0)=0$, i.e., the photovoltage is zero at $t=0$.

For not very heavily doped semiconductors, the contribution of the processes of thermionic emission and tunneling to the restoring current J can be best described by the thermionic-field-emission current J_{tf}.[2] As a good approximation, the restoring current can be written as

$$J=J_{tf}+J_{rec}+J_{le}, \tag{5}$$

where J_{rec} is the current due to the carrier recombination within the depletion region[2] and J_{le} is the leakage current.[3] In the steady-state situation, a steady-state photovoltage V_0 is produced for the photocurrent J_{pc0} and J_{pc0} and V_0 should satisfy the equation below:

$$J_{pc0}-J(V_0)=0. \tag{6}$$

In the present work, as an example, we study the metal/n-GaAs contacts. The parameters used in the calculation are: the relative dielectric constant $\epsilon_r=13.1$, the Richardson constant $A^*=8.6\times10^4$ A m^{-2} K^{-2}, the lifetime of the carriers $\tau=10^{-6}$ s, the de-ionized energy of the dopant $E_d=0.006$ eV, the effective mass of electrons is $0.067m_e$, and the values of the pulse width t_a and the pulse delay t_b of the square wave of $J_{pc}(t)$ are set to be $t_a=t_b=1$ s.

The transient characteristics of the photovoltage at different temperatures are shown in Fig. 1. At 50 and 100 K it takes about 3 s for the photovoltage to grow from zero to the steady-state value V_0 (see the dashed curves); however, at 300 K, it takes about 10^{-6} s to complete this process. This situation is actually due to thermionic emission. As required by Eq. (6), for the same V_0 the photocurrent $J_{pc0}(=3.1\times10^{-3}$ A cm$^{-2})$ at 300 K is much larger than that at 100 and 50 K (J_{pc0} is 6.0×10^{-9} A cm^{-2} at both the temperatures). The photocurrent behaves as a charging current, and a larger charging current leads to a shorter charging time; thus, the rising time of the photovoltage is shorter for a larger photocurrent. On the other hand, the decay of the photovoltage at 300 K is much faster than that at 50 and 100 K. This situation arises because thermionic emission, which is more important at higher temperatures, can speed up the discharging process. Figure 1 shows the consequences: At 300 K the wave form of the "output" (i.e., the photovoltage) is almost identical to that of the "input" (i.e., the photocurrent); however, at both 50 and 100 K the wave form of the "output" is distorted and the photovoltage cannot reach its steady-state value V_0. As can be seen in Fig. 1, the transient characteristics is insensitive to temperature at low temperatures (say, $T<100$ K). This is because thermionic emission

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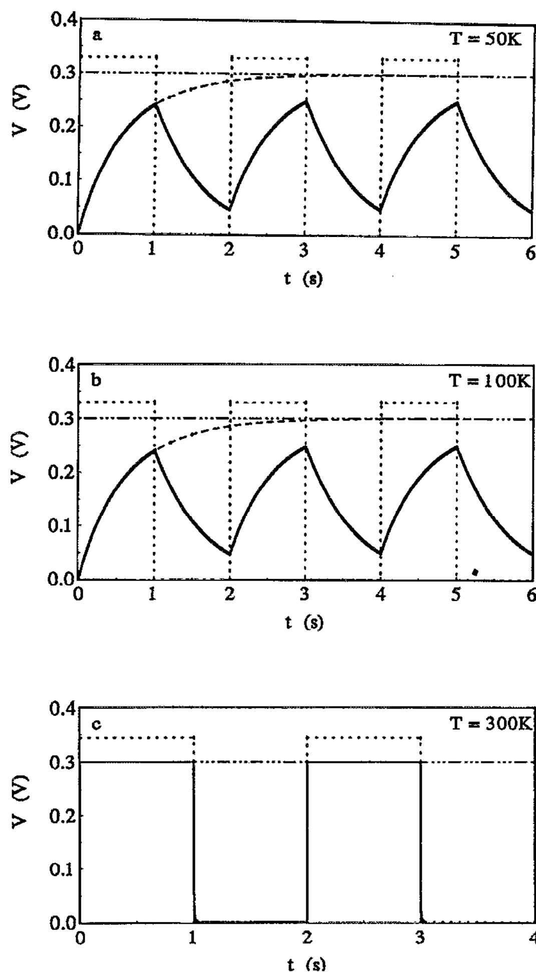

FIG. 1. Temperature dependence of the transient characteristics of the photovoltage under the conditions of $N_d=1\times10^{15}$ cm^{-3}, $q\Phi_b=0.80$ eV, and $R=1\times10^8$ Ω (the solid curves). The dashed curves represent the growth of the photovoltage from zero to the steady-state value $V_0(=0.30$ V), and the dotted lines represent the variation of the photocurrent $J_{pc}(t)$. (a) $T=50$ K, $J_{pc0}=6.0\times10^{-9}$ A cm^{-2}; (b) $T=100$ K, $J_{pc0}=6.0\times10^{-9}$ A cm^{-2}; and (c) $T=300$ K, $J_{pc0}=3.1\times10^{-3}$ A cm^{-2}.

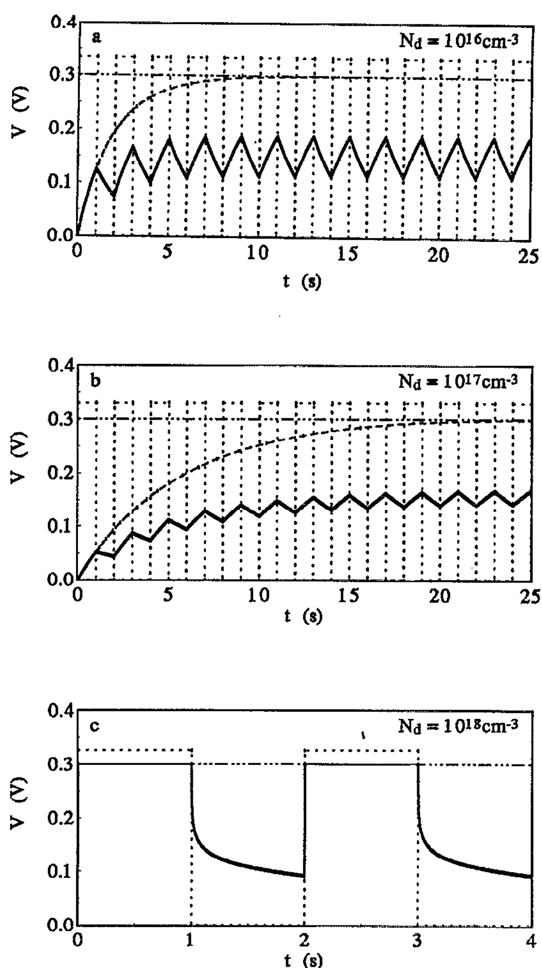

FIG. 2. Doping-concentration dependence of the transient characteristics of the photovoltage under the conditions of $T=150$ K, $q\Phi_b=0.80$ eV, and $R=1\times10^8$ Ω (the solid curves). The dashed curves represent the growth of the photovoltage from zero to the steady-state value $V_0(=0.30$ V) and the dotted lines represent the variation of the photocurrent $J_{pc}(t)$. (a) $N_d=1\times10^{16}$ cm^{-3}, $J_{pc0}=6.0\times10^{-9}$ A cm^{-2}; (b) $N_d=1\times10^{17}$ cm^{-3}, $J_{pc0}=6.3\times10^{-9}$ A cm^{-2}; and (c) $N_d=1\times10^{18}$ cm^{-3}, $J_{pc0}=9.0\times10^{-5}$ A cm^{-2}.

is greatly suppressed and other current transport mechanisms, such as tunneling and leakage which are independent of temperature, become more significant at low temperatures.

The effect of the doping concentration of the semiconductor on the transient characteristics is shown in Fig. 2. Compared to the lower doping concentrations (for example, $N_d=1\times10^{16}$ cm^{-3}), the higher doping concentration $N_d=1\times10^{18}$ cm^{-3} leads to a much shorter rising time and a shorter decay time for the photovoltage. It is well known that, as the doping concentration increases, the Schottky barrier becomes thinner and, thus, the tunneling current is larger.[2] Therefore, as shown in Eq. (6), for the same V_0, a larger photocurrent J_{pc0} is required for a larger doping concentration. A large photocurrent will speed up the charging process and thus shorter rising time is obtained. On the other hand, when the photovoltage decays upon the cessation of the illumination, the tunneling effect also speeds up the discharging process leading to a shorter decay time; however, it should be pointed out that the effect of tunneling on the transient characteristics is obvious only for high doping concentrations ($N_d\geqslant1\times10^{18}$ cm^{-3}). For low doping concentrations, increase of doping concentration does not lead to a shorter rising and decay time. This situation can be seen through the comparison of Figs. 2(a) ($N_d=1\times10^{16}$ cm^{-3}) and 2(b) ($N_d=1\times10^{17}$ cm^{-3}). As shown by the dashed curves in Figs. 2(a) and 2(b), the growth of the photovoltage from zero to V_0 takes about 10 s, for $N_d=1\times10^{16}$ cm^{-3} but it takes about 23 s for $N_d=1\times10^{17}$ cm^{-3}. The reason for this situation is that the doping concentration has two opposing effects on the transient characteristics. As the doping concentration increases, both the capacitance of the contact junction [see Eq. (3)] and the influence of the tunneling effect increase, but, the former will increase the rising and decay time while the later will reduce them. For low doping concentrations, the former effect will be more dominant and thus a

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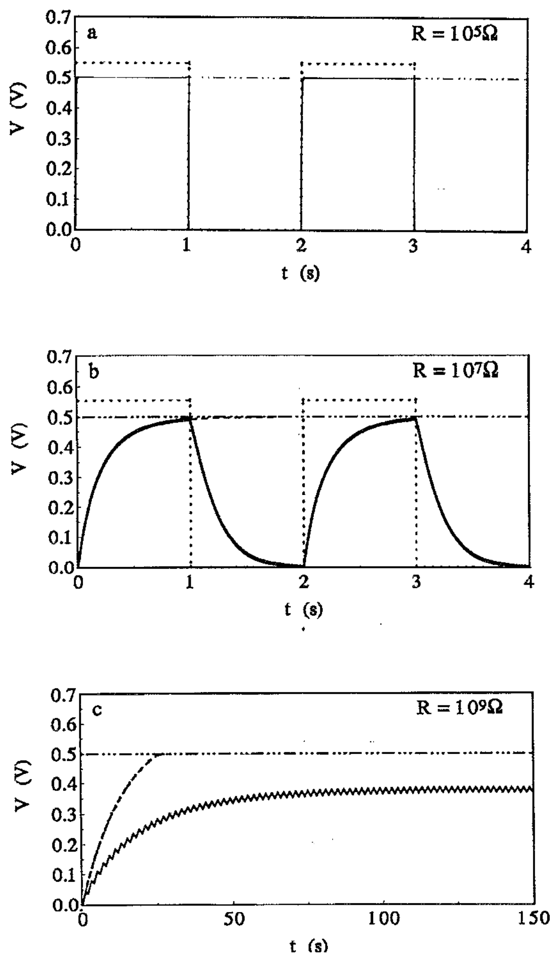

FIG. 3. Leakage-resistance dependence of the transient characteristics of the photovoltage under the conditions of $T=100$ K, $N_d=1\times10^{16}$ cm^{-3}, and $q\Phi_b=0.80$ eV (the solid curves). The dashed curves represent the growth of the photovoltage from zero to the steady-state value $V_0(=0.50$ V) and the dotted lines represent the variation of the photocurrent $J_{pc}(t)$. (a) $R=1\times10^5$ Ω, $J_{pc0}=1.0\times10^{-5}$ A cm^{-2}; (b) $R=1\times10^7$ Ω, $J_{pc0}=1.0\times10^{-7}$ A cm^{-2}; and (c) $R=1\times10^9$ Ω, $J_{pc0}=1.5\times10^{-9}$ A cm^{-2}.

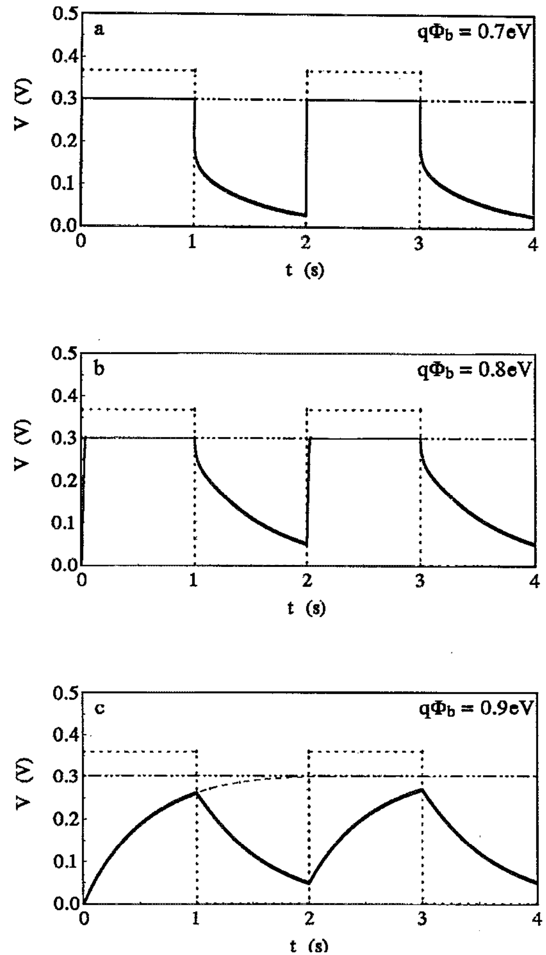

FIG. 4. Schottky-barrier-height dependence of the transient characteristics of the photovoltage under the conditions of $T=200$ K, $N_d=1\times10^{15}$ cm^{-3}, and $R=1\times10^8$ Ω (the solid curves). The dashed curve represents the growth of the photovoltage from zero to the steady-state value $V_0(=0.30$ V) and the dotted lines represent the variation of the photocurrent $J_{pc}(t)$. (a) $q\Phi_b=0.70$ eV, $J_{pc0}=4.0\times10^{-5}$ A cm^{-2}; (b) $q\Phi_b=0.80$ eV, $J_{pc0}=1.4\times10^{-7}$ A cm^{-2}, and (c) $q\Phi_b=0.90$ eV, $J_{pc0}=6.5\times10^{-9}$ A cm^{-2}.

higher doping concentration will lead to a longer rising time and decay time.

Figure 3 demonstrates the significant effect of the leakage current on the transient characteristics of the photovoltage. For the leakage resistance $R=1\times10^5$ Ω [Fig. 3(a)], the current transport is dominated by the leakage current, and the rising time and decay time for the photovoltage are about 0.01 s; for $R=1\times10^7$ Ω [Fig. 3(b)], the leakage current is not dominant but still significant, and the rising time and decay time are about 1 s; as the leakage resistance increases to 1×10^9 Ω [Fig. 3(c)] the leakage current is no longer significant and the rising time and decay time are limited by the thermionic-field emission which leads to the noiselike behavior of the transient photovoltage (note that the photovoltage can never reach its steady-state value V_0).

Figure 4 shows the effect of barrier height on the transient characteristics of the photovoltage. Based on the thermionic-emission theory[2] the thermionic emission depends on barrier height, and a higher barrier height will lead to a smaller thermionic-emission current. Therefore, for a given V_0 the J_{pc0} decreases with increasing $q\Phi_b$ as required by Eq. (6), and the decrease of J_{pc0} slows down the charging process leading to a longer rising time of the photovoltage. On the other hand, the decrease of the restoring current J due to the increase of barrier height also slows down the discharging process, and thus a longer decay time of the photovoltage is obtained for a higher barrier height.

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