Deep-level delta doping of Ti in GaAs: Modeling of tunnel-assisted recombination

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The tunnel-assisted recombination current of a thin GaAs *pn* junction delta doped with Ti deep-level defects is modeled by 1D device simulation using a generalized Shockley–Read–Hall rate. The tunneling between band states and multiphonon sublevels of the recombination center, and the Poole–Frenkel effect are studied, varying the position of the delta-doped sheet and the junction width. Both field effects decisively influence the calculated current-voltage characteristics.

The performance of most electronic devices is influenced by recombination via deep-level defects. In *pn* junctions, the recombination depends on the local position of the deep center corresponding to the deviation of the local carrier concentrations $n(x)$ and $p(x)$ from equilibrium. In most cases, little is known about the nature of the dominant deep-level defect. The description of the recombination of electrons and holes is based on the Shockley–Read–Hall (SRH) statistics.[1] Recently,[2] the SRH recombination was generalized to include the effect of inhomogeneous electric fields. Specifically, the interaction of multiphonon and tunneling transitions in *one* recombination process was described. Here, pure thermal (fixed position) and pure tunnel (fixed energy) transitions appear as borderline cases for zero field and zero temperature, respectively. Each step of the thermally induced carrier capture into deep centers can be assisted by tunneling between band-edge states and the levels of the "phonon ladder" (Fig. 1). This leads to a position-dependent carrier lifetime $\tau(x)$, even for a homogeneous center distribution, reflecting the spatial variation of the electric field and thereby of the tunneling probability. When the recombination centers are introduced in a delta-doped thin sheet within the space-charge region of *pn* junctions, the tunnel-assisted multiphonon transitions become well separated, since there is only one phonon ladder that is related to the center's energy E_r at a given position. We have analyzed this behavior with the one-dimensional device simulation routine PC-1D[3] that has been extended to calculate the lifetimes of delta-doped deep level recombination according to Ref. 2.

For the following discussion of a practical example, we assume delta doping of an abrupt GaAs *pn* junction with titanium. Ti doping of III-V semiconductors yields semi-insulating material and has the advantage of low diffusivity compared to other transition metal impurities. Thus, the recombination properties of Ti in GaAs and InP are currently of particular interest.[4–6] In the band gap of GaAs, substitutional Ti causes two deep levels:[4] the $\mathrm{Ti}^{2+}/\mathrm{Ti}^{3+}$ acceptor level at $E_c-0.20$ eV that acts as an electron trap, having a neutral charge state when not occupied, and a negative state when occupied. Its cross section for electron capture at high temperature is $s_n^\infty \approx 3\times10^{-16}$ cm^2 and is hardly changed at room temperature.[5] The $\mathrm{Ti}^{3+}/\mathrm{Ti}^{4+}$ donor level at $E_c-0.87$ eV is neutral when occupied by an electron or positively charged when empty. The cross sections for this state at room temperature are $s_n\approx10^{-14}$ cm^2 for electron capture, and $s_p\approx10^{-15}$ cm^2 for hole capture. In *p*-type GaAs, both Ti levels are not occupied by electrons. Here, the donor state of Ti is positively charged and acts as a strong capturing center for electrons. The acceptor-like charge state of Ti can be neglected for recombination if located at the junction interface or within the *p* region.[7]

Hence, in the following calculations, a delta-doped sheet of Ti donor levels is assumed at different local positions within the *p* side of the junction. For the density of shallow donors and acceptors, a value of $N_d=N_a=2\times10^{17}$ cm^{-3} is used in order to generate a built-in electric field that is high enough for significant tunneling. A delta-doping density of 10^{10} cm^{-2} is chosen that is low enough for quantum-well effects to be negligible, but high enough that recombination-induced changes in the device characteristics can be distinguished. Such a relatively low doping density does not cause a marked step of the electric field *F*. Electron capture by the donor level involves the effect of Coulomb barrier lowering. We apply the one-dimensional Poole–Frenkel model neglecting screening by free carriers, which is justified in depletion regions: $\Delta E_r = -\sqrt{qF/\pi\epsilon_0\epsilon}$. As individual center parameters, we spec-

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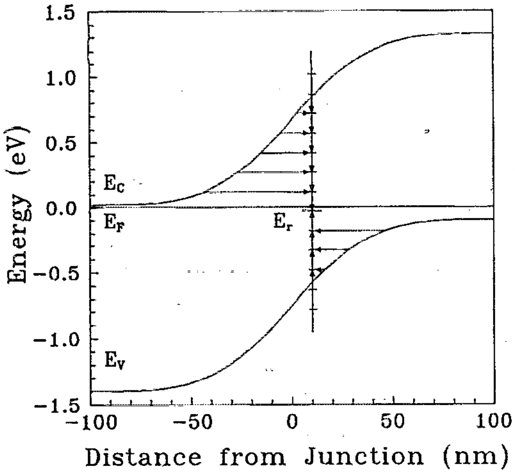

FIG. 1. Energy-band diagram of an abrupt GaAs *pn* junction ($N_d=N_a=2\times10^{17}$ cm^{-3}) at zero bias with conduction band edge E_c, valence-band edge E_v, Fermi level E_F, and the donor-like Ti level ($E_r=E_c-0.87$ eV) that is incorporated by delta doping within the *p* region. The arrows indicate tunnel-assisted recombination paths (the plotted level spacing of the phonon ladder is schematically drawn and does not match the assumed value of $\hbar\omega_0=33$ meV).

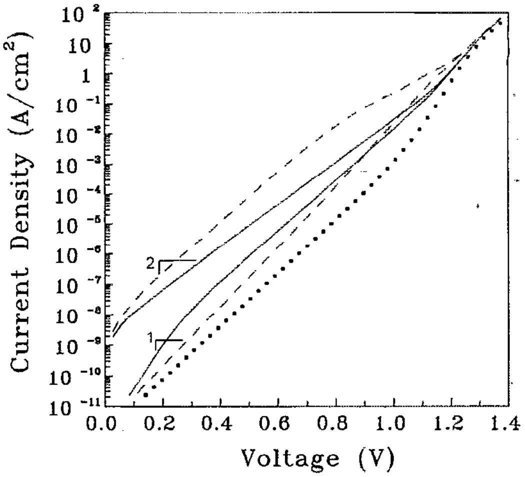

FIG. 3. Computed *jV* characteristics of the GaAs *pn* junction with the delta-doped deep donor-like level at the junction interface (solid), 10 nm shifted into the *p* region (dashed) and without deep level (dotted): (1) classical current, (2) tunnel-assisted recombination with Poole–Frenkel effect.

ify an effective phonon energy $\hbar\omega_0=33$ meV and a lattice relaxation energy $S\ \hbar\omega_0$ with $S=3.5$. The model uses adjustable parameters that are determined by fitting the current density versus voltage (*jV*) characteristics at tunnel-free center positions outside the space-charge region to the classical PC-1D results (calculated with the measured capture cross sections).

Figure 2 shows the classical forward *jV* characteristic in comparison to the currents that are influenced by the Poole–Frenkel shift, by tunnel-assisted recombination, and by both effects, for a Ti sheet at a distance of 10 nm from the metallurgical junction interface. At low forward bias, tunnel-assisted recombination (curve 3) dominates the current-voltage characteristic, whereas with increasing forward bias (decreasing field strength), the Poole–Frenkel effect (curve 2) starts to dominate. This behavior is modified depending on the actual electric field at the center that can be altered by a variation of the local sheet position, or by changing the shallow dopant concentration. *jV* characteristics with and without field-induced effects on the lifetimes are given in Fig. 3 for two different positions of the deep-level sheet. Without field enhancement (curves 1), the recombination increases as the sheet approaches the junction interface. At higher forward bias, however, a crossover occurs because the energy differences between the deep level and the quasi-Fermi levels depend on the local center position.[7] Taking into account tunneling and Poole–Frenkel effects (curves 2), the recombination center becomes more effective when it is shifted by several nm from the junction interface into the *p* region. The deep-level position at 10 nm results in a larger current than when the center is located at the interface. This behavior is related to the different electric field distribution around the deep centers and can be explained as follows. At the given doping density, the built-in field has a maximum value of about 2×10^5 V/cm in the middle of the junction and decreases by about 3 kV/cm per nm distance from the junction interface. At the left of the centers the electric field determines the electron tunneling, at the right it controls the hole tunneling (see Fig. 1). Electron tunneling into the center at 10 nm inside the *p* region (dashed curve 2 in Fig. 3) is more supported by the field distribution than with the delta-doped sheet at the junction interface (solid curve 2 in Fig. 3). Which recombination path is most likely depends on both the probabilities of tunneling and phonon release. With the center at 10 nm, the electron tunneling length with maximum capture rate is 13–14 nm, for holes only about 4 nm. On the other hand, with the delta-doped layer

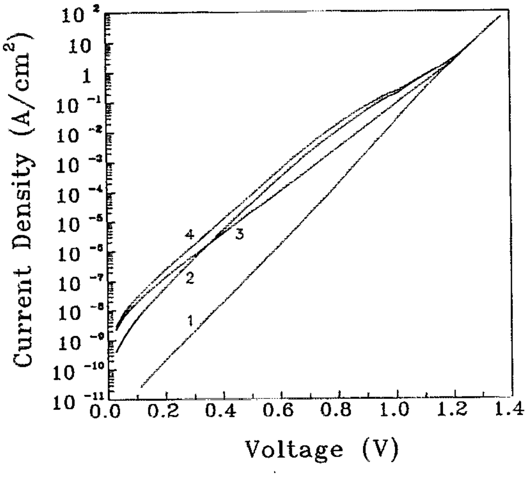

FIG. 2. Calculated *jV* characteristics of the GaAs *pn* junction with the deep donor-like level delta doped in the *p* side at a distance of 10 nm from the interface: (1) Classical current without field effects, (2) classical current with Poole–Frenkel effect, (3) tunnel-assisted current without Poole–Frenkel effect, and (4) current with both field effects.

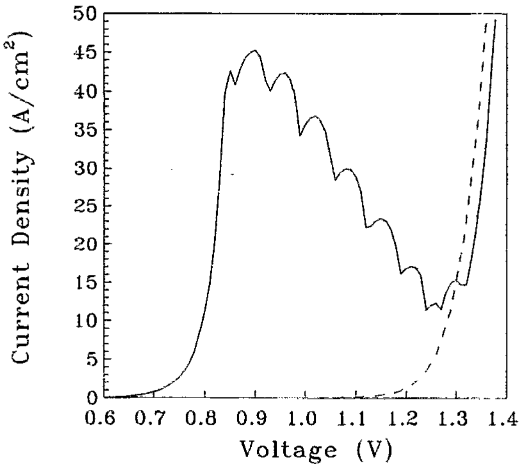

FIG. 4. High-voltage part of the jV characteristic with the center in the middle of the junction for a shallow dopant density of $N_d = N_a = 10^{19}$ cm^{-3} (solid) and $N_d = N_a = 2 \times 10^{17}$ cm^{-3} (dashed), respectively.

at the junction interface, the prefered electron tunneling length decreases to 11–12 nm.

Higher concentrations of shallow dopants raise the built-in electric field maximum and reduce the Debye length. With the deep center at the interface of an abrupt GaAs *pn* junction doped by $N_d = N_a = 10^{19}$ cm^{-3} shallow impurities, a seven times higher field leads to a 500 times higher maximum tunnel current and a sawtooth-like jV characteristic (Fig. 4) as predicted in Ref. 2. The origin of this extraordinary jV shape is the exclusion of sublevel after sublevel of the "phonon ladder" from the tunneling process with increasing forward bias (see Fig. 1). The tunneling peaks shown in Fig. 4 are not as sharp as in Ref. 2 because the tunneling rate of the borderline phonon level decreases due to the field lowering at higher voltages before this tunnel path disappears. The tunnel dips occur at voltages V_i at which the *i*th phonon level is crossing the energy position of the corresponding majority carrier band edge at the space-charge boundary. That means for holes with the center in the middle of the junction: $qV_{ip} = qV_{bi} - 2(E_r - E_v - i\hbar\omega_0)$ with V_{bi} being the built-in voltage ($V_{bi} = 1.427$ V for $N_d = N_a = 10^{19}$ cm^{-3}, $E_r - E_v = 0.55$ eV). These V_{ip} values match the dip positions in Fig. 4 up to high voltages, indicating that hole tunneling is the "bottleneck" recombination process and that it determines the sawtooth-like structure (near the flatband case the employed Schottky approximation is no longer valid). If the tunneling current would be dominated by electrons, dips would occur at somewhat higher voltages $V_{in} = V_{bi} - 2(E_c - E_r - i\hbar\omega_0)/q$. In both cases, the V_i spacing is $2\hbar\omega_0/q = 0.066$ V as to be seen in Fig. 4. When the electric field is almost vanishing near the flatband case, the tunneling is switched off at all as soon as no more sublevels of the phonon ladder can be reached from the band edges. This happens for hole tunneling at 1.38 V forward bias, for electron tunneling at 1.40 V. At these voltages, the total jV characteristic (solid curve in Fig. 4) is already dominated by carrier diffusion.

In conclusion, tunnel-assisted recombination and Poole–Frenkel effect can have a significant influence on the recombination properties of the Ti center within a space-charge layer in GaAs. This could change substantially the current-voltage characteristic in forward bias.

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