Enhancement of deep acceptor activation in semiconductors by superlattice doping

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The thermal activation of acceptors in wide-gap semiconductors can be very low due to large acceptor activation energies. It is shown that superlattice doping, i.e., the composition modulation of a uniformly doped ternary semiconductor, can enhance the acceptor activation by more than one order of magnitude. © *1996 American Institute of Physics.*
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The achievement of high p-type conductivity in many wide-band gap semiconductors has been shown to be difficult due to the large acceptor binding energies.[1] In the case of III–V nitrides, the acceptor effective Rydberg energies are 200–400 meV for commonly used acceptors such as Mg and Zn.[2] In the freeze-out regime, the free hole concentration in a semiconductor with acceptor concentration N_A and acceptor binding energy E_a is given by[3]

$$p=\sqrt{\frac{1}{g}\,N_A N_V}\,\exp\left(-\frac{E_a}{2kT}\right), \tag{1}$$

where g is the acceptor degeneracy, N_V is the effective density of states at the valence band edge, and kT is the thermal energy. For an acceptor energy of 200 meV, the electrical activation calculated from Eq. (1) is 6% at room temperature.[4]

To overcome the fundamental problem of low acceptor activation, we propose a uniformly doped ternary compound semiconductor structure with a spatially modulated chemical composition. The modulation of the chemical composition leads to a variation of the valence band energy. It will be shown in this publication that the modulation of the valence band results in a strong enhancement of the acceptor activation. The free carrier properties of composition-modulated structures will be calculated and discussed.

The band diagram of a uniformly doped, composition-modulated semiconductor structure is shown in Fig. 1(a). It is assumed that the acceptor effective Bohr radius is much smaller than the period of the superlattice, so that the acceptor levels in the barriers are not influenced by adjacent wells and vice versa (see, for example, Ref. 5). For an effective mass of $m_h^*=0.8\ m_0$, the effective Bohr radius calculated for hydrogenic impurities is 6 Å, i.e., much smaller than the period of the superlattice discussed here. Figure 1(b) schematically shows the free carrier concentration in the valence band. The hole concentration is modulated and follows the modulation of the valence band edge.

The calculations of the one-dimensional semiconductor model were performed on an (SGI) Power Challenge 18 processor computer system. Fermi-dirac statistics was used for the acceptor and valence band occupancy. The band edge energies, free carrier concentration, and the acceptor activation were calculated as a function of depth. The compositional modulation used in the computations was either abrupt or parabolically graded. GaN material parameters were used for the calculations.[7] The modulation of the composition was assumed to be small.[8]

We consider the case of a square-shaped valence band modulation. A doping concentration of $N_A=1\times10^{18}\ \text{cm}^{-3}$ and an acceptor activation energy of $E_a=200$ meV are used in the calculation. The magnitude of the valence band modulation used in the calculation is given by $\Delta E_V=E_a=200$ meV. The free carrier concentration along with the doping concentration are shown in Fig. 2. The free carrier concentration reaches $10^{18}\ \text{cm}^{-3}$ in the wells demonstrating very high activation of the deep acceptors. The effective carrier concentration, defined as the arithmetic average over the period of the structure, is $5\times10^{17}\ \text{cm}^{-3}$. Thus the effective activation of the acceptor impurities is 50%. The effective concentration is nearly a factor of ten higher than the concentration of an unmodulated semiconductor with the same material parameters, where a free carrier concentration inferred from Eq. (1) is $5.5\times10^{16}\ \text{cm}^{-3}$, corresponding to an activation of 6%. The higher doping activation in the modulated structure will result in higher conductivity in particular for transport in the planes of the modulated layers.

Very high electrical activation of deep acceptors can be achieved, if the acceptor energy levels in the barriers are

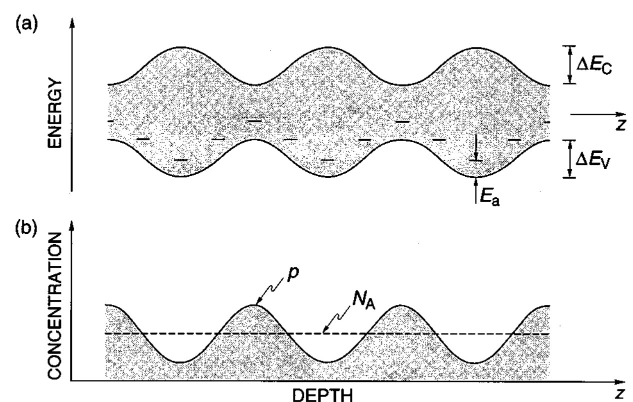

FIG. 1. (a) Schematic band diagram of a ''straddled lineup'' semiconductor superlattice with a modulated chemical composition. (b) Doping concentration N_A, and hole concentration p.

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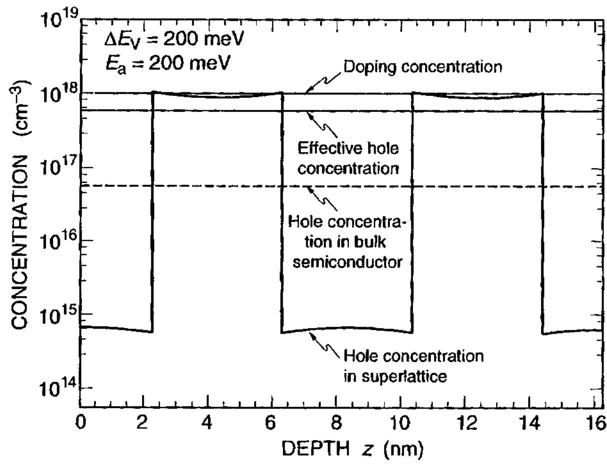

FIG. 2. Calculated hole concentration in a semiconductor superlattice with a modulated valence band energy. The structure is uniformly doped at $N_A = 1\times10^{18}$ cm^{-3}. Also shown is the *effective hole concentration* ($p_{\text{eff}}=5\times10^{17}$ cm^{-3}) which is the hole concentration averaged over one period. The dashed line shows the hole concentration ($p=5.5\times10^{16}$ cm^{-3}) in a bulk semiconductor without composition modulation doped at $N_A=1\times10^{18}$ cm^{-3}.

energetically close to the valence band states in the wells. This condition can be written as

$$\Delta E_V - E_a \geqslant E_{0h} + (E_F - E_{0h}) + E_{\text{dipole}}, \quad (2)$$

where E_{0h} is the energy of the lowest quantized state relative to the top of the valence band, ($E_F - E_{0h}$) is the band filling of the valence band states, and E_{dipole} is the energy due to the polarization of the material (band bending). The latter energy is given by twofold integration of Poisson's equation

$$E_{\text{dipole}} = -\frac{e^2}{\varepsilon}\int_0^{(z_p/2)}\int_0^{z}[p(z') - N_A^-(z)]d_{z'}dz, \quad (3)$$

where z_p is the period of the structure. The period of the structure is chosen small enough to make band bending effects negligible and large enough (well thickness >30 Å for $m_h^* = 0.8m_e$) to make confinement effects negligible.

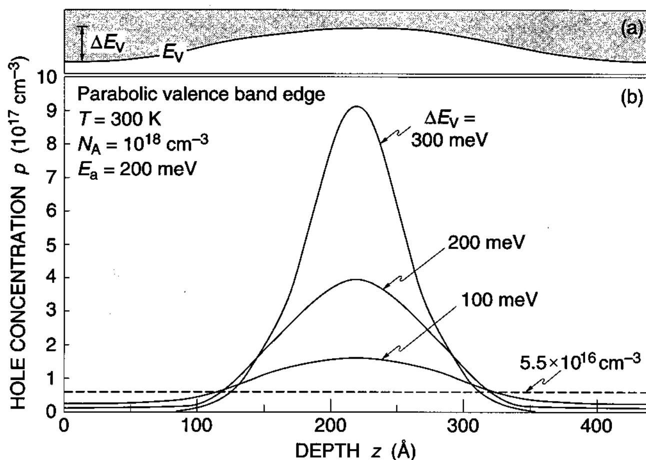

FIG. 3. Hole concentration in a parabolically graded structure for different magnitudes of the valence band modulation ΔE_V. Also shown is the carrier concentration in a bulk semiconductor (dashed line) with the same acceptor concentration and activation energy.

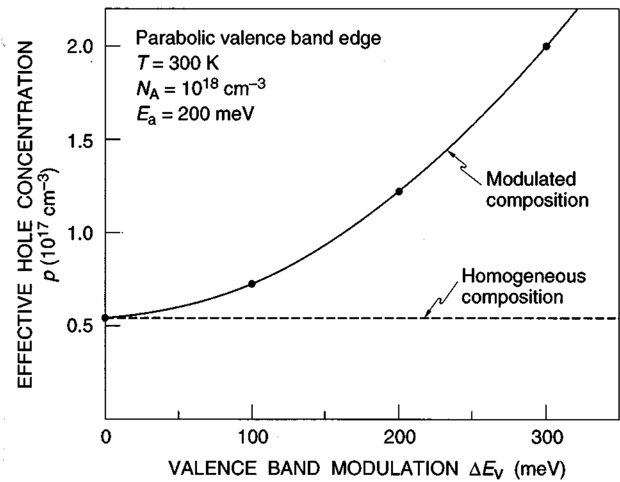

FIG. 4. Effective hole concentration of a parabolically graded structure as a function of the valence band modulation.

A useful figure of merit is the *acceptor activation efficiency* which is defined as

$$\eta = \frac{p_{\text{eff}}}{N_A} = \frac{1}{N_A}\frac{1}{z_p}\int_0^{z_p} p(z)dz. \quad (4)$$

The efficiency approaches unity for large barriers and narrow wells if the condition of Eq. (2) is fulfilled. Efficiencies >85% are calculated for asymmetric structures with a barrier-to-well width ratio of 8:1. This activation efficiency corresponds to an increase by more than a factor of ten when compared to an unmodulated structure. Note that the structures discussed here are uniformly doped. Diffusion of impurities is therefore irrelevant assuming that the diffusion coefficient in the barriers and wells is the same.

We next discuss the free carrier concentration in parabolically graded structures. The curvature of the parabolically graded region is chosen in such a way that the electrostatic depletion potential of ionzied acceptors in the barriers is similar to the valence band modulation caused by the compositional modulation. This method was shown to result in low resistances for transport across the barriers when compared to interfaces with abrupt composition changes.[9]

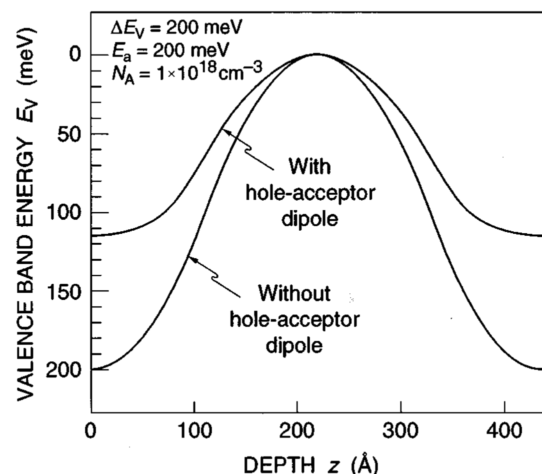

FIG. 5. Valence band modulation with and without taking into account the band modulation caused by hole and acceptor charges.

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The calculated free carrier concentration of three parabolically graded structures are shown in Fig. 3. The magnitude of the modulation is $\Delta E_V = 100$, 200, and 300 meV. The structure has a period of $z_p = 400$ Å. Figure 3 shows free carrier peak concentrations as high as $\approx 10^{18}$ cm^{-3} for the largest band modulation.

The effective free carrier concentration of the parabolically graded structure is shown in Fig. 4 for the three different band modulations. The carrier concentration of the unmodulated structure is shown for comparison. For the highest band modulation ($\Delta E_V = 300$ meV), a 3.6 times higher carrier concentration is obtained.

The band modulation of the parabolically graded structure with $\Delta E_V = 200$ meV is shown in Fig. 5. Both the unperturbed band modulation and the modulation reduced by the electrostatic dipole potential are shown. The spatial separation of ionized acceptors and holes leads to a reduction of the valence band modulation. The residual modulation is approximately 115 meV. If the potential modulation caused by the charge dipole becomes comparable to the magnitude of the band modulation, a decrease in acceptor activation results.

In conclusion, we showed that the electrical activation of acceptors in wide-gap semiconductors can be enhanced by superlattice doping, i.e., by modulating the composition of a doped semiconductor. For a modulation equal to the acceptor binding energy ($\Delta E_V = E_a = 200$ meV), a more than ten-fold increase of the free carrier concentration from 5.5×10^{16} to 8.5×10^{17} cm^{-3} is calculated for a short-period (<100 Å) abrupt modulation. In addition, parabolically graded structures were discussed which have reduced resistance for transport across the interfaces. A 3.6 times increase of the free carrier concentration was calculated for parabolically graded structures.

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[4] The parameters used in the calculation are $g = 2$, $N_A = 1 \times 10^{18}$ cm^{-3}, $N_V = 1.8 \times 10^{19}$ cm^{-3}, and $E_a = 200$ meV. The effective density of states, N_V, is calculated from the parabolic band model using the GaN effective hole mass of $m_h^* = 0.8 m_0$.

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[6] The assistance of the Center for Computational Science at Boston University is acknowledged.

[7] The materials parameters included $m_h^* = 0.8 m_0$, $N_V = 1.8 \times 10^{19}$ cm^{-3}, $E_a = 200$ meV, $T = 300$ K, $\varepsilon_r = 9.0$.

[8] A *small* modulation of the composition will leave the semiconductor ''GaN-*like*.'' The effective density of states (N_V) and the acceptor binding energy (E_a) are therefore taken to be constant, i.e., independent of the composition. Impurity activation energies in ternary III–V nitrides were reviewed in Ref. 2. More experimental data would be required to take into account the possible composition dependence of the acceptor activation energy. The corrections to the results presented here would, however, be minor.

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