Quantum-well reshaping by hot electrons in planar-doped structures

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The self-consistent calculations of the potential well in a planar-doped semiconductor demonstrate that carrier heating in strong electric fields leads not only to a repopulation of the two-dimensional carriers between the subbands but also to a significant deepening and broadening of the quantum well, which is accompanied by a change of the subband energies consequently. The important role of such a change is confirmed by the particularities of the formation of metastable DX^- centers in planar-doped GaAs:Si.

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Treating the problem of hot electrons in semiconductors it is usually taken for granted that the electron heating does not influence their energy spectrum, but only changes the carrier distribution among the energy levels. This assumption was also used in all studies, in which the heating of two-dimensional (2D) electrons confined in potential wells created by planar doping has been investigated already for more than a decade.[1–3] However, since the quantum well in a δ-doped semiconductor depends on the space charge distribution in a self-consistent way, it therefore has to depend on the carrier distribution among the energy levels. Indeed, the population of higher subbands caused by strong electric fields leads to an electron distribution which is more extended in space, and as a consequence the well becomes broader and deeper. It is obvious that the electron temperature, at which this effect becomes significant, depends on the doping concentration.

To elucidate this idea we performed a model calculation solving the system of the one-dimensional Schrödinger and Poisson equations—complemented by the neutrality condition—numerically by an iteration method for different temperatures and doping concentrations. In dimensionless variables ($L_0=\hbar^2\varepsilon/me^2$, $E_0=me^4/\varepsilon^2\hbar^2$, and $N_0=1/L_0^2$, with ε denoting dielectric permittivity) they are

$$\frac{d^2\Psi_n(x)}{dx^2}+2[E_n-V(x)-V_{ex}(x)]\Psi_n(x)=0, \quad (1)$$

$$\frac{d^2V(x)}{dx^2}=4\pi\left\{N_s\delta(x-x_0)-\frac{T}{\pi}\times\sum_n \ln\left[1+\exp\left(-\frac{E_n-\mu}{T}\right)\right]|\Psi_n(x)|^2\right\}, \quad (2)$$

$$N_s-\frac{T}{\pi}\sum_n \ln\left[1+\exp\left(-\frac{E_n-\mu}{T}\right)\right]=0. \quad (3)$$

V_{ex} and μ are the exchange and correlation and Fermi energy, respectively, T denotes the temperature in dimensionless energy units, x_0 the position of the doped plane, and N_s the concentration of doping atoms in this plane. The corresponding boundary conditions are

$$V(\infty)=0, \quad \Psi_n(\infty)=0,$$

$$\frac{dV(0)}{dx}=2\pi N_s,$$

$$\Psi_n(0)=0 \quad \text{if } n \text{ even},$$

$$\frac{d\Psi_n(0)}{dx}=0 \quad \text{if } n \text{ odd}.$$

In zeroth order the potential was analytically obtained from the Poisson equation by the Thomas-Fermi approximation. In the following iterations we included the exchange and correlation energy in local density approximation into the Schrödinger equation in the form given in Ref. 4. The electron transfer into 3D states was omitted[14] and the nonparabolicity was neglected. The carrier distribution among the subbands in the potential well was assumed to be a Fermi distribution (as one can see from the used form of the Poisson equation). As such a type of distribution is only valid for the equilibrium state, strictly speaking we calculate the temperature dependence of the potential at zero applied field strength. But most likely such a substitution is justified since the self-consistent potential does not depend on the lattice temperature explicitly, while the temperature in the Fermi function denotes an electron temperature. As for high electron concentrations in δ-doped layers even at heating electric fields the electron-electron interaction is dominant among the inelastic scattering processes, which are responsible for the energy distribution, a Fermi distribution with an effective electron temperature can be introduced as a possible approximation. The connection between the electron temperature and the electric field has to be determined then separately, usually by a Monte Carlo simulation or a numerical solution of the Boltzman equation. Of course, it strongly depends on the lattice temperature.

The necessary parameters $m_{\rm eff}=0.067m_0$ and $\varepsilon=12.8$ were chosen for GaAs as an example. The calculations were performed as far as 150 nm from the doping plane; for a distance up to 30 nm the interval between two neighboring points was chosen equal to 0.125 nm, further on equal to 0.5 nm. The self-consistent calculation was continued until the potential in each of all the 480 points did not change any-

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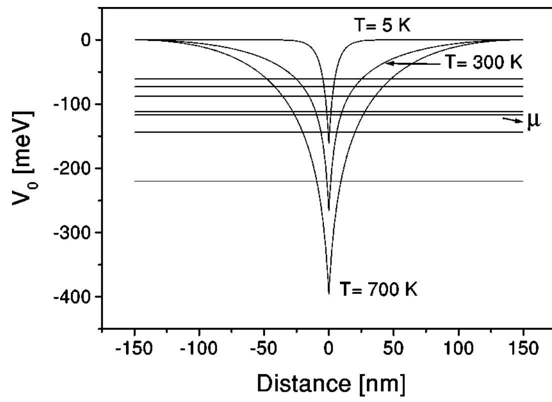

FIG. 1. Self-consistently calculated potential for electron temperatures of 5, 300, and 700 K. δ-doped GaAs:Si with a doping concentration of $5\times10^{12}\ \mathrm{cm}^{-2}$.

more within an accuracy of 0.1%. The number of energy levels in the potential well was cut off automatically by the prescription that the highest-energy level taken into account did not deviate from zero energy by more than several percent of the considered electron temperature. Between 30 and 600 iterations were necessary, the number depending on temperature and concentration.

The potential well with $5\times10^{12}\ \mathrm{cm}^{-2}$ donors, which was obtained integrating the Poisson equation, is shown for 5, 300, and 700 K in Fig. 1. For 300 K the energy levels are included as lines, the Fermi level being at 117 meV. The curve for 5 K is in good agreement with the known data, e.g., for thermal equilibrium at 4.2 K; cf. Fig 1.4 in Ref. 5. As claimed in the beginning Fig. 1 shows that the width and depth of the potential well depend on the electron temperature in a pronounced way. In Fig. 2 the calculated well depth normalized to its value for $3\times10^{12}\ \mathrm{cm}^{-2}$ in dependence on concentration is shown for 5, 77, and 500 K. We see that the higher the temperature the weaker is this normalized dependence as could be expected for physical reasons. Figure 3 demonstrates the dependence of the potential well depth on carrier temperature for concentrations of 4, 7, and 12.5 $\times10^{12}\ \mathrm{cm}^{-2}$. The results are normalized to their respective low-temperature limits to exhibit the essential trend that the dependence on temperature is weaker for the more doped material as expected.

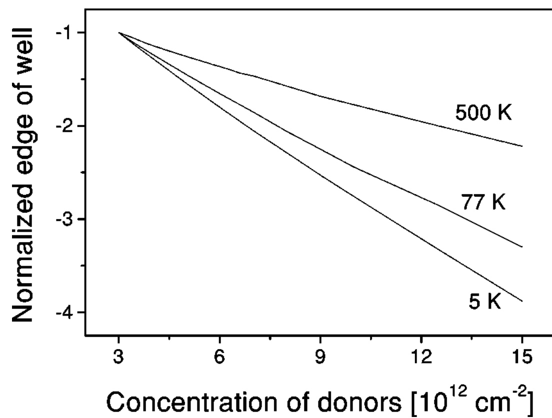

FIG. 2. Concentration dependence of the potential well depth normalized to the value for a concentration of $3\times10^{12}\ \mathrm{cm}^{-2}$ calculated for electron temperatures of 5, 77, and 500 K. The normalizing values are 5 K–105 meV, 77 K–128 meV, and 500 K–265 meV.

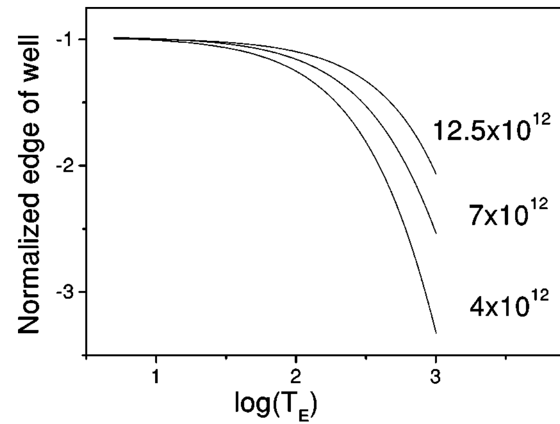

FIG. 3. Dependence of potential well depth on electron temperature normalized to the values at 5 K calculated for donor concentrations of $4\times10^{12}\ \mathrm{cm}^{-2}$, $7\times10^{12}\ \mathrm{cm}^{-2}$, and $12.5\times10^{12}\ \mathrm{cm}^{-2}$. The normalizing values are 133, 214, and 347 meV, respectively.

We used these results to understand some peculiarities of the metastable DX^{-}-center formation in planar-doped GaAs:Si in heating electric fields.[6,7] Such a center can be described as a substitutional $\mathrm{Si}_{\mathrm{Ga}}$ atom shifted to an interstitial site with two bound electrons.[8–10] By an application of a heating electric field DX^{-} centers can be formed and this leads to a decrease of the carrier concentration (and of the 2D current) with time. An example of the time dependence of the resulting current change is shown for different field strengths at a lattice temperature of 77 K in Fig. 4.[15]

One of the peculiarities of DX^{-}-center formation in planar-doped GaAs:Si is that it becomes implemented only if the concentration of dopants exceeds a value of about 4

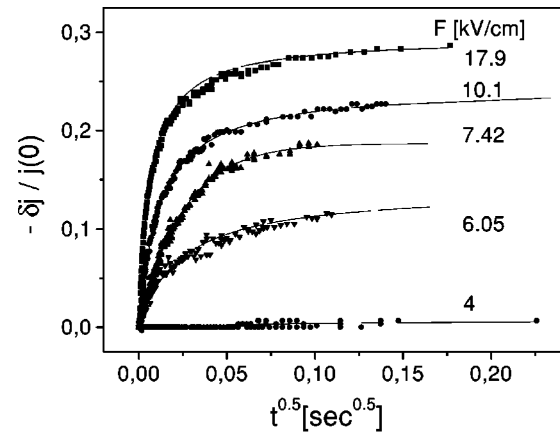

FIG. 4. Normalized current change versus duration of applied fields for GaAs:Si planar doped with $7\times10^{12}\ \mathrm{cm}^{-2}$ atoms [initial electron concentration according to Shubnikov–de Haas oscillations (Ref. 6) equal to $5\times10^{12}\ \mathrm{cm}^{-2}$]: the symbols denote experimentally determined values; the lines present the results of fitting procedures.

$\times 10^{12}$ cm^{-2}. This concentration is much higher than that of the equivalent value for volume doping at which DX^- centers were observed (10^{17} cm^{-3}). Further on there is a well-expressed threshold with respect to the field, at which the formation of DX^- centers can be obtained. Then with growing field strength the current change increases until a saturation is gained (30% change as maximum). The existence of the threshold is clearly demonstrated in Fig. 4, where at a field strength of 4 kV/cm a current change is almost absent.

There are different models of DX^--center formation. But in each of them it becomes realized only if the wave function of the conduction electrons at the energy of the resonant metastable state is concentrated in the vicinity of the doping atoms in order to warrant that the interaction between electrons and lattice is strong enough to lead to a displacement of the doping atom from its lattice site. For a planar-doped semiconductor it means that the resonant energy level has to be positioned within the potential well. Taking a resonant level energy of about 280 meV as known from experimental investigations in GaAs[11,12] we conclude (see Fig. 3) that at electron temperatures lower than 180 K for a sample like the one in Fig. 4 the resonant level is positioned above the potential well. Heating the electrons at a lattice temperature of 77 K by an electric field the potential well becomes deeper and at a certain field strength the resonant level dips into the well. Then the formation of DX^- centers becomes possible.

We do not intend to analyze the conditions for the formation of DX^- centers in planar-doped semiconductors in this short paper in detail, but only want to confirm that the deepening of the potential well in heating electric fields permits to explain the thresholds concerning concentration and heating fields. Their existence is essential for the physics of DX^- centers in planar-doped semiconductors and can be understood in the framework of the proposed model in a reasonable way. It would be interesting to investigate how the self-consistent change of the quantum well influences other processes in heating electric fields. It is particularly desirable to repeat a calculation of the electron energy distribution as a function of field strength,[1] taking the self-consistency of the problem into account.

We would also like to mention that the change of the potential well in a heating electric field can take place in other semiconductor structures, too, for instance, in heterostructures with inversion layers such as Si/SiO_2, and should be considered.

In conclusion we would like to note that electron heating can be implemented not only by an electric dc field. Especially infrared light may be used for this purpose.[13] Then the change of the energy spectrum of a planar-doped semiconductor can lead to various nonlinear effects.

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[14] The validity of this assumption depends on the electron temperature and number of 3D states related to the single doped plane. A simple estimation proves that if the distance between doped planes is smaller than 250 nm, the filling of 3D states is negligible for $T \leqslant 1000$ K.

[15] We use square-root scale for time to represent the short and long-time regions of curves more or less adequately.