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Photoionization threshold of the deep donor in Si-doped $Al_xGa_{1-x}As$

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In order to clear up the controversy about the magnitude of the lattice relaxation of the deep donor in n-type $Al_xGa_{1-x}As$, samples were exchanged between Philips and IBM. The present photocapacity study on an IBM sample definitely shows the existence of two photoionization processes: one with a threshold between 200 and 300 meV, representing an effective-mass-type deep donor with small lattice relaxation, and another one with a threshold near 700 meV, representing the so-called DX center with large lattice relaxation. These results suggest either two distinct donor configurations or a bistable character of the deep donor.

Recent photoluminescence studies[1,2] of n-type $Al_xGa_{1-x}As$:Si revealed the existence of four donor levels D_1, D_2, D_3, and D_4, in order of increasing ionization depth. The number of donor levels and the dependence of their ionization energies on the Al fraction x follows qualitatively the predictions of the generalized effective-mass theory.[3,4] The deepest donor level D_4 is tied to the L minimum of the conduction band. This property and the magnitude of its ionization energy (200 meV with respect to the L minimum) suggests an identification with the DX center known from electric measurements.[5] One marked difference, however, throws doubts on this identification. The DX center is believed to exhibit a large lattice relaxation responsible for the thermal barriers for emission and capture.[5-7] The deep donor D_4, on the other hand, shows a small lattice relaxation, as evidenced by the phonon structure of the D_4A luminescence[8] (Huang-Rhys figure of $S=0.5$ and coupling to LO phonons with $\hbar\omega=48$ meV) and the small value of the Stokes shift.[9]

Additional information on the magnitude of the lattice relaxation can be obtained from the threshold of the photoionization cross section. The small lattice relaxation (SLR) model predicts a threshold of the order of the thermal depth (about 200 meV), whereas the large lattice relaxation (LLR) model allows a threshold of the order of 1 eV. Experimental determinations of the photoionization threshold by means of photocapacity and photoconductivity measurements have recently been reported by Legros, Mooney, and Wright[10] and by Henning and Ansems.[11] The results, however, are controversial. Legros *et al.*[10] report a threshold of about 850 meV, pointing to large lattice relaxation, whereas the present authors[11] find a threshold near 225 meV, in accordance with the SLR model.

In order to figure out the origin of the discrepancy it was decided to exchange samples. The Philips sample (807, $x=0.33$) used in Ref. 11 has recently been remeasured by the IBM group. For $0.8<\hbar\omega<1.5$ eV, the shape of the photoionization cross section agrees with the one reported in Ref. 11. Below 0.8 eV, however, no transient photocapacitance signals could be observed.[12] In the present paper, we report a photocapacitance study of one of the IBM samples (NH 321, $x=0.74$) used in Refs. 10 and 12.

The sample was grown by molecular-beam epitaxy (MBE) on an n^+-type GaAs substrate. A thin buffer layer of GaAs was followed by a graded $Al_xGa_{1-x}As$ layer 0.3 μm in thickness in which x increased gradually from 0 to the desired value 0.74. The active layer of $Al_{0.74}Ga_{0.26}As$ has a thickness of 0.7 μm. Schottky contacts (In or Au) were applied to the top of the active layer and an Ohmic contact (Sn) was mounted at the substrate side. The Si concentration was such that $N_d-N_a=7.0\times10^{16}$ cm^{-3}. In addition, deep-level transient spectroscopy (DLTS) measurements[13] revealed a deep trap at $E_c-E_T=0.87\pm0.04$ eV, with a concentration of $N_T=1.5\times10^{16}$ cm^{-3}. Illumination occurred via the substrate side of the specimen. The light source consisted of a Nernst glower followed by a set of interference and semiconductor filters. The filter combination had a bandwidth of about 10 nm for $500<\lambda<1300$ nm, 100 nm for $1.5<\lambda<3$ μm, and 150 nm for $\lambda>3.5$ μm. The photon flux was measured with a laser precision power meter (RL 3610) with an average accuracy of 3%. The capacity of the Schottky diode was measured at 1 MHz by a Boonton (type 72 B) capacity meter; the dark value of the capacity at $T=35$ K was approximately 20 pF. The output of the Boonton bridge was connected either to a storage oscilloscope (Gould OS 4100) to record fast transients, or to a pen recorder, for slow transient phenomena.

Since the application of light may alter the distribution of carriers among the various traps more or less permanently, one should stringently adhere to a well-defined measurement procedure. After thermalization at $T=300$ K, the sample was cooled to 35 K at a prescribed cooling rate. The light was turned on (at $t=0$) and the photocapacity transient was recorded until an equilibrium state was reached. No bias voltage was applied either during cooling or during the measurement. After turning off the light the decay towards the final state was recorded. Finally, the sample was heated up again to 300 K.

As a consequence of the strong temperature dependence of the capture cross section, the number of filled deep donors depends on the cooling rate; it can be described by an effective filling factor f $(0<f<1)$: $N^0(t=0)=fN$, N being the donor concentration. In our experiments, f could be reproduced to within a few percent. For a center in the depletion layer of a metal-semiconductor junction the filling factor is also a function of position $f(x)$; here, $x=0$ refers to the point where band bending starts and $x=W$ refers to the metal layer. Although emission processes dominate in the middle of the space-charge region, recapture from free carrier tails cannot be neglected in regions close to the boundaries of this volume.[14,15] This is especially important when capacity measurements are made at zero-bias voltage. The rate equations then read

$$dN^+/dt=\sigma_n^0\phi N^0-c_n n(x,t)N^+ , \quad (1)$$

where $n(x,t)$ is the free-electron density, N^0 and N^+ are the densities of filled and ionized donors, respectively, ϕ is the photon flux, σ_n^0 the absorption cross section, and c_n the electron capture coefficient. In the small signal approximation $[\Delta n<N^+(x,0)]$, Eq. (1) can be linearized and rewritten in terms of $\Delta n=n(x,t)-n(x,0)=N^+(x,t)-N^+(x,0)$:

$$d\Delta n/dt=\sigma_n^0\phi f(x)N-\sigma_n^0\phi\Delta n-\Delta n/\tau \quad (2)$$

with

$$1/\tau=c_n[1-f(x)]N+c_n n(x,0) . \quad (3)$$

For fixed x, the solution to Eq. (2) is a simple exponential. Its stationary value is given by

$$\Delta n(x,\infty)=\frac{\sigma_n^0\phi f(x)N-c_n n(x,0)[1-f(x)]N}{\sigma_n^0\phi+c_n[1-f(x)]N+c_n n(x,0)} . \quad (4)$$

When $f(x)=1$, the final value $\Delta n(x,\infty)$ is proportional to the total density N. This does not always hold true if $f(x)<1$. Assuming compensation $[n\ll(1-f)N]$, two extreme cases can be distinguished. If $\sigma_n^0\phi>c_n(1-f)N$, the final value is again proportional to N:

$$\Delta n(x,\infty)\simeq f(x)N . \quad (4a)$$

If, however, $c_n(1-f)N>\sigma_n^0\phi$, $\Delta n(x,\infty)$ is no longer a measure of N:

$$\Delta n(x,\infty)\simeq\frac{\sigma_n^0\phi f(x)}{c_n[1-f(x)]} . \quad (4b)$$

The initial slope is directly read from the differential equation (2):

$$[d(\Delta n)/dt]_{t=0}=\sigma_n^0\phi f(x)N . \quad (5)$$

The light-induced change in the occupation of the centers leads to a change in the junction capacity. Since the test frequency (1 MHz) exceeds the emission rate at $T=35$ K, the traps cannot follow the test signal and the capacity is determined by the movement of electrons at the edge of the depletion layer. The change dW of the width of the depletion layer, caused by an occupation change $\Delta n(x,t)$ in a infinitesimal volume between x and $x+dx$ is obtained by solving the Poisson equation twice, remembering that the experiment is carried out at constant bias voltage. The macroscopic capacity change then follows from an integration over the depletion layer[14]

$$\Delta C/C=\frac{1}{n_0W^2}\int_0^W\Delta n(x,t)(W-x)dx , \quad (6)$$

n_0 being the bulk carrier density. If we further make the simplifying assumption that $f(x)=f$ for $0<x<\lambda$, and $f(x)=0$ elsewhere, a combination of Eqs. (4a), (4b), and (5) with Eq. (6) gives

$$\frac{\Delta C_\infty}{C}=\frac{fN}{2n_0}\frac{2W\lambda-\lambda^2}{W^2}\quad[\sigma_n^0\phi>c_n(1-f)N] , \quad (7a)$$

$$\frac{\Delta C_\infty}{C}=\frac{f\sigma_n^0\phi}{2(1-f)c_n n_0}\frac{2W\lambda-\lambda^2}{W^2}\quad[\sigma_n^0\phi<c_n(1-f)N] , \quad (7b)$$

$$1/C(dC/dt)_{t=0}=\frac{f\sigma_n^0\phi N}{2n_0}\frac{2W\lambda-\lambda^2}{W^2} . \quad (8)$$

The point λ corresponds to the crossing of the electron quasi-Fermi level with the deep-donor level.

The experimental results are summarized in Figs. 1 and 2. They clearly show that photocapacity transients are observable below $\hbar\omega=800$ meV. The threshold for photoionization is found somewhere between 200 and 300 meV, at variance with the results of Legros *et al.*[10] and of Mooney *et al.*,[12] but in agreement with Ref. 11 [see, however, Ref. 16]. For $\hbar\omega<600$ meV the transients are fast. The stationary value is reached within a second and remains constant on a longer time scale. The shape of the transients is exponential [Figs. 1(a)–1(c)]. The observation that for small ϕ both the initial slope and the final value of the transient are proportional to ϕ shows that the

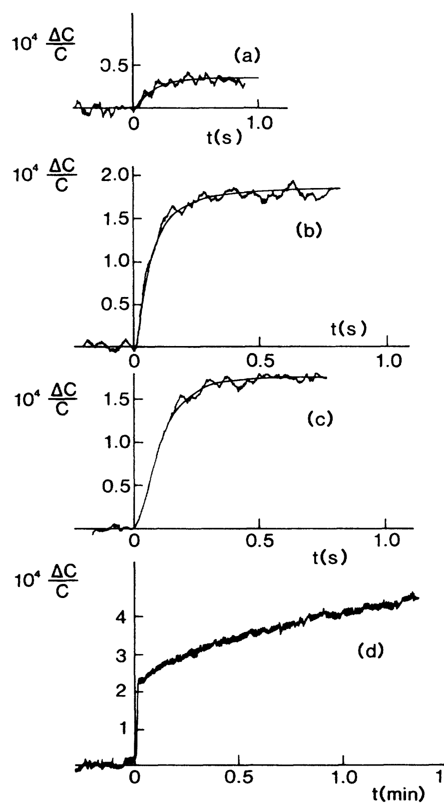

FIG. 1. Photocapacity transients of $Al_{0.74}Ga_{0.26}As$:Si (IBM sample NH 321) at $T=35$ K. (a) $\hbar\omega=283$ meV, $\phi=2.42\times10^{15}$ cm^{-2}s^{-1}. (b) $\hbar\omega=352$ meV, $\phi=2.96\times10^{15}$ cm^{-2}s^{-1}. (c) $\hbar\omega=523$ meV, $\phi=2.96\times10^{15}$ cm^{-2}s^{-1}. (d) $\hbar\omega=728$ meV, $\phi=4.87\times10^{15}$ cm^{-2}s^{-1}.

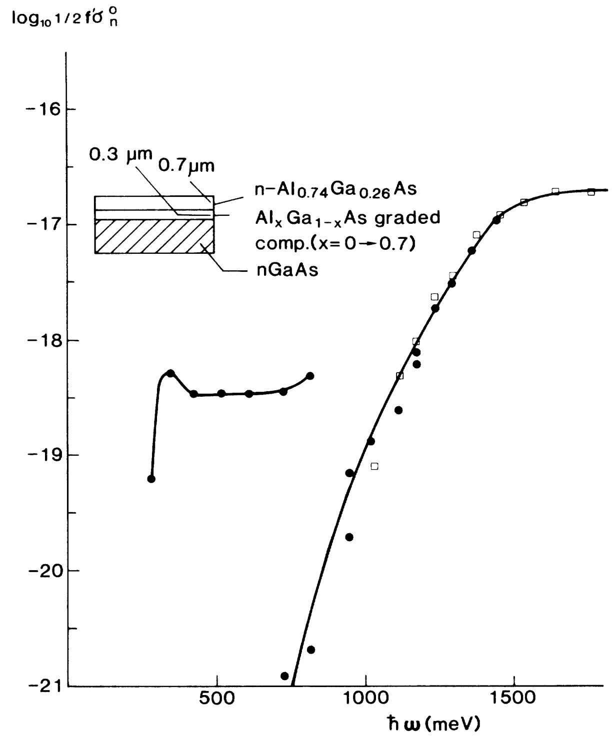

FIG. 2. Photoionization cross section, as deduced from photocapacity transients for $Al_{0.74}Ga_{0.26}As$ (NH 321). Black dots, present work. Open squares, Legros *et al.* (Ref. 10) at $T=82$ K, normalized to our data at $\hbar\omega=1.45$ eV. $f'=f(N/n_0)(2W\lambda-\lambda^2)/W^2$.

approximations $\Delta n < N^+$ and $\sigma_n^0\phi < c_n(1-f)N$ are appropriate to this case. The amplitudes of the transients therefore do not reflect the donor density. If we divide the initial slope by the final value we arrive at a constant value for 0.28 eV $<\hbar\omega<$ 0.82 eV, in agreement with Eqs. (7b) and (8). The value of the constant is $(1-f)c_nN=(6\pm 1)\ \mathrm{s}^{-1}$.

For $\hbar\omega>700$ meV, a second, slower photoionization process sets in [Fig. 1(d)]. The slower process dominates when $\hbar\omega>800$ meV. For 700 meV $<\hbar\omega<820$ meV both the fast and the slow photoionization processes occur simultaneously [see Figs. 1(d) and 2]. A decomposition into two exponential transients is readily made. The spectral distribution of the relative absorption cross sections for both processes is presented in Fig. 2. The $\sigma_n^0(\hbar\omega)$ curve for the slow process agrees well with the data of Legros *et al.*[10] (open squares in Fig. 2). Its threshold is around 700 meV.

The shape of the absorption curve of the fast (low-energy) process deviates appreciably from a Lucovsky profile.[17] This might be due to the fact that the depletion layer in this moderately doped sample is not restricted to the active layer with well-defined $x=0.74$, but extends into the graded intermediate layer. Moreover, photoionization of the donor level D_3, with mixed L and X character is expected to occur in the same spectral region.[2]

Persistent photocapacity effects are found to occur for $\hbar\omega>650$ meV, which might suggest that this phenomenon is related to the onset of the slow photoionization process.

To summarize, the present photocapacity study of a relatively clean, MBE-grown $Al_{0.74}Ga_{0.26}As$:Si sample definitely shows the existence of two photoionization processes with thresholds around 200–300 meV and 700 meV, respectively. The lower threshold is in perfect agreement with the predictions of the small lattice relaxation model for the D_4 donor level.[8] The assignment to $D_4\rightarrow L$ (and possibly also $D_3\rightarrow L$) transitions seems the most natural one since photoluminescence spectra of this sample show D_4A (at 2.129 eV) and D_3A (at 2.087 eV) as the most conspicuous features at low temperature. Moreover, DLTS measurements[13] do not reveal any other impurities apart from DX and a midgap center (at 0.87 eV). The higher threshold represents the well-known DX center, with large lattice relaxation. The present results seem to indicate that the incorporation of Si gives rise to either two distinct donor sites or to a donor with a bistable ground state. Further experiments are needed to distinguish between these two possibilities.

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