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Equivalence of donor and acceptor fits to temperature-dependent Hall data: General case

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Recently, it was shown that the usual statistical-mechanical formulation used to fit carrier concentration versus temperature data cannot distinguish between the donor or acceptor nature of one single-charge-state center. Here we generalize that result to include any number of donor and acceptor centers, of arbitrary charge multiplicity, and also show how that by fitting one particular case (e.g., every center assumed to be a donor), all of the other possible cases can be immediately solved by inspection.

A common method to determine donor and acceptor concentrations and energy levels in a semiconductor is to fit temperature-dependent Hall-effect data with the charge-balance equation, derived from statistical mechanics.^{1,2} Very recently, we showed³ that such a fit cannot distinguish between the donor or acceptor nature of *one single-charge-state* center, even though the charge-balance equations for the donor and acceptor cases appear to be different. The main purpose of the present work, which should be considered an addendum to Ref. 3, is to give a general proof of the equivalence of donor and acceptor fits for all cases, including multicharge centers. It is shown in Ref. 4 that the generalized "charge-balance" equation for arbitrary donor and acceptor species (each designated by k) is

$$n = p + \sum_{\substack{k,l,m \\ l_k = 0 \text{ for } A}} (l_k - l)n_{klm}, \quad (1a)$$

where l_k is the number of electrons ionizable from the neutral state ($l_k = 0$ if center k is a pure acceptor), l ranges from zero to the maximum change of electron occupation, and

$$n_{klm} = N_k \left(1 + \sum_{l',m' \neq l,m} \frac{g_{kl'm'}}{g_{klm}} \right)^{-1} \times \exp\{[\epsilon_{klm} - \epsilon_{kl'm'} - (l - l')\epsilon_F]/k_B T\} \quad (1b)$$

The index m denotes excited states, and the summation restriction is that $l \neq l'$ and $m \neq m'$ at the same time. Note that the only asymmetry between donors and acceptors in Eq. (1a) is the factor l_k , which is the total number of electrons that donor center k may release from its neutral state (with the final electron still requiring less than band-gap energy for ionization). For pure donors, the summation index l will range from 0 to l_k , while for pure acceptors, $l_k = 0$, and l ranges from 0 to the number of electrons that acceptor center k may trap onto its neutral state. Consider, e.g., a triple donor, for which $l_k = 3$ and $l = 0, 1, 2, 3$ and compare that with a triple acceptor, for which $l_k = 0$ and $l = 0, 1, 2, 3$. To make the acceptor appear as a donor in the last term of Eq. (1a), we simply define an acceptor l_k to equal the maximum l for the acceptor, and then add and subtract equal terms in Eq. (1a). Formally,

$$\begin{aligned} n &= p + \sum_{\substack{k,l,m \\ l_k = 0 \text{ for } A}} (l_k - l)n_{klm} \\ &= p + \sum_{\substack{k,l,m \\ \text{all } A,D}} (l_k - l)n_{klm} - \sum_{\substack{k,l,m \\ A}} l_k n_{klm} \\ &= p + \sum_{\substack{k,l,m \\ \text{all } A,D}} (l_k - l)n_{klm} - \sum_k l_k N_k, \end{aligned} \quad (2)$$

where now the only asymmetry between donors and acceptors is in the last term of Eq. (2). But the last term is *temperature independent* and thus will simply add to the temperature-independent part of the next-to-last term, which arises from the "shallow" centers, both donors (N_{DS}) and acceptors (N_{AS}), whose occupations do not change over the temperature range of the experiment. However, the major parameters of an n -vs- T fit, namely, the concentrations, energy levels, and degeneracy factors of the *principal* centers, come from the *temperature-dependent* parts of the next-to-last term and are not affected by the absence or presence of the last term. [To show this, we simply need to take a temperature derivative of Eq. (2) and fit that equation, instead.] Then, since the next-to-last term is independent of any particular center's donor or acceptor nature, the proof is complete.

To illustrate, we consider a case in which there are four single-charge-state ($l_k = 1$) centers, C_1 , C_2 , C_3 , and C_4 . Over the temperature range of interest, C_2 and C_3 have variable occupation factors, whereas C_1 is a donor of concentration N_{DS} , lying well above ϵ_F at all temperatures, and C_4 is an acceptor of concentration N_{AS} , lying well below ϵ_F . Then, with the excited-state index m suppressed, Eq. (2) becomes

$$\begin{aligned} n &= p + \sum_{k=2,3} n_{k0} + K \\ &= p + \sum_{k=2,3} \frac{N_k}{1 + (g_1/g_0)_k e^{-\alpha_k/k_B (E_{k0} - E_F)/k_B T}} + K, \end{aligned} \quad (3)$$

where now the energies are defined with respect to the conduction band, and α_k is defined by $E_k = E_{k0} - \alpha_k T$. The fitted parameters are N_k , E_{k0} , $(g_1/g_0)_k \exp(-\alpha_k/k_B)$, and K , for $k = 2, 3$. Note that the first three parameters are inde-

TABLE I. Interpretation of constant K in Eq. (6) ($N_1 \equiv N_{DS}$ and $N_4 \equiv N_{AS}$).

C_2	C_3	K
D	D	$N_{DS} - N_{AS}$
D	A	$N_{DS} - N_{AS} - N_3$
A	D	$N_{DS} - N_{AS} - N_2$
A	A	$N_{DS} - N_{AS} - N_2 - N_3$

pendent of the donor or acceptor nature of C_2 and C_3 . However, the definition of K changes, as shown in Table I, and

since N_2 and N_3 are already determined from the fit, $N_{DS} - N_{AS}$ can be immediately calculated for each case.

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Effect of interface structure on photoluminescence of InGaAs/GaAs pseudomorphic single quantum wells

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Photoluminescence studies have been carried out on InGaAs pseudomorphic single quantum wells grown on GaAs by molecular beam epitaxy. Linewidths as narrow as 2.0 meV have been observed. The spectra typically consist of two peaks which on certain samples can be explained by intrawell thickness variations of one monolayer. On other samples the results are more consistent with exciton trapping at islands having a smaller lateral extent than the exciton Bohr radius.

In recent years there has been considerable interest in the use of photoluminescence (PL) as a means of investigating the interface quality of quantum well (QW) structures. One aspect of this work has been the demonstration of multiple peaks in the PL spectrum due to intrawell thickness variations in GaAs/AlGaAs QW's.¹⁻⁴ These are observed when the diameters of the stepped regions are larger than the diameter of the exciton. Interruption of the growth at the interface, leading to a smoothing of the surface, has been shown to give this condition. In QW's grown without interruption, a single wide peak is generally observed. This peak is often Stoke's shifted to lower energies due to trapping of the excitons at regions where the QW is wider, but the lateral extent is smaller than the exciton Bohr radius.

The InGaAs/GaAs strained-layer materials system is coming under increasing investigation due to its promising device potential in both optoelectronics and in field effect transistor structures.⁵ InGaAs pseudomorphic QW's have generally shown inferior linewidths compared to equivalent GaAs/AlGaAs structures and have therefore been of limited use for interface studies. In principle, the absence of the relatively rough AlGaAs surface in these structures should eliminate the problem of asymmetric interfaces. However, other effects, such as indium segregation, could possibly complicate the situation. In this communication we present

PL spectra from pseudomorphic InGaAs single QW's with linewidths narrow enough such that trapping effects are clearly visible.

The samples were grown by molecular-beam epitaxy (MBE) on (100)-oriented semi-insulating GaAs substrates. Both As₄ and As₂ (from a cracker cell) were employed, with typical As/Ga beam equivalent pressure ratios of 10 and 4, respectively. Indium-free mounting was used for all the substrates. The indium concentration (x_{In}) in the QW's is typically 15%–20%. In all cases a GaAs buffer layer of at least 1 μ m was deposited before the QW, followed by a 600 Å capping layer. The buffer layer and QW structure were grown at 640 and 520 °C, respectively. The growth rate was obtained from thick calibration layers. The luminescence was obtained using the conventional lock-in technique with a 0.5-m Jarrel-Ash monochromator. The excitation source was a HeNe laser with a typical excitation intensity ~ 1 W cm⁻². All measurements were carried out at 5 K using a continuous flow cryostat. The spectra obtained were curve fitted using the Levenberg-Marquardt method⁶ and the best fit chosen by minimizing a chi-square merit function.

Figure 1 shows the PL spectrum at ~ 5 K obtained from a QW with $L_z = 73$ Å and $x_{In} \sim 0.17$, together with the spectrum generated by the curve-fitting procedure. The experimental curve is seen to be closely fitted by a superposition of