Magneto-Transport Characterization Using Quantitative Mobility-Spectrum Analysis

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A quantitative mobility spectrum analysis (QMSA) of experimental Hall and resistivity data as a function of magnetic field is presented. This technique enables the conductivity contribution of bulk majority carriers to be separated from that of other species such as thermally generated minority carriers, electrons, and holes populating n and p doped regions, respectively, and twodimensional species at surfaces and interface layers. Starting with a suitable first trial function such as the Beck and Anderson mobility spectrum analysis (MSA), a variation on the iterative procedure of Dziuba and Gorska is used to obtain a mobility spectrum which enables the various carrier species present in the sample to be identified. The QMSA algorithm combines the fully automated execution and visually meaningful output format of MSA with the quantitative accuracy of the conventional least-squares multi-carrier fitting procedure. Examples of applications to HgCdTe infrared detector materials and InAs/GaSb quantum wells are discussed. The ultimate goal of this paper is to provide an automated, universal algorithm which may be used routinely in the analysis and interpretation of magneto-transport data for diverse semiconductor materials and bandgap engineered structures.

Key words: HgCdTe, Hall measurements, mobility spectrum analysis, transport properties

INTRODUCTION

Mixed-conduction effects nearly always have a strong influence on the magneto-transport properties of narrow bandgap infrared (IR) semiconducting materials such as HgCdTe.¹ Multiple species due to n and p doped regions, thermally generated minority carriers, and two-dimensional populations at surfaces and interface layers tend to make significant contributions to the conduction process in addition to the bulk majority carriers. Standard measurements of the resistivity and Hall coefficient at a single magnetic field are of limited use when applied to systems with prominent mixed-conduction, since they

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provide only averaged values of both the carrier concentration and mobility, which may not necessarily be representative of any of the individual carrier species. Far more information becomes available if the magneto-transport experiments are performed as a function of magnetic field because, in principle, the data can then be deconvolved in order to obtain densities and mobilities for each carrier species present in the sample.¹⁻³

Traditionally, the conventional technique for analyzing magnetic-field-dependent Hall data is the multicarrier fitting (MCF) procedure.² However, this technique requires prior assumptions to be made about the number of electron and hole species as well as their approximate mobilities. As a result, injudicious guesses can often lead to misleading and/or ambiguous results. In order to overcome this shortcoming, Beck and Anderson proposed a novel approach known as mobility spectrum analysis (MSA),⁴ in which an envelope of the maximum conductivity is determined as a continuous function of carrier mobility. While MSA is a fully automated procedure that provides a visually meaningful output format, the information provided by the technique is primarily qualitative rather than quantitative. In particular, it is not possible to obtain a fit to the actual experimental Hall and resistivity data.

In an attempt to overcome these difficulties, Meyer et al.¹ have developed and extensively tested a hybrid mixed conduction analysis (HMCA) procedure, in which the MSA spectrum is used initially to determine the number of carrier species and to roughly estimate their densities and mobilities, and the MCF is then used to obtain a final quantitative fit. The second stage of that procedure is not automated, and results can be expressed only in terms of a discrete number of carrier species with discrete mobilities.

In this work, we discuss the implementation of a quantitative mobility spectrum analysis (QMSA) procedure, which preserves both the visually meaningful output format of the Beck and Anderson MSA technique and the quantitative accuracy of the conventional least-squares MCF result; yet the procedure is entirely automated. The present approach is a variation on the iterative fitting procedure originally developed by Dziuba and Gorska.⁵

Unlike mobility spectrum analysis, which derives only an envelope of the maximum carrier density which may be present with a given mobility, the spectra obtained from this numerical formalism are adjusted so as to optimize the quantitative agreement with the experimental results. The ultimate goal of this work is to develop a comprehensive and fully automated method for quantitatively analyzing and interpreting magneto-transport data; a universal algorithm which is suitable for widespread use as an industry standard. We will address the issues which need to be resolved before this objective can be achieved.

We begin the exposition with brief descriptions of the conductivity tensor for multicarrier systems in the next section and the multi-carrier fitting procedure in the section of that title. In the section on mobility spectrum, we describe the Beck and Anderson MSA and the iterative approach of Dziuba and Gorska. Details of the QMSA approach are then given in the same section.

The Results and Discussion section presents and discusses illustrative results, using the examples of an InAs/GaSb single quantum well grown by molecular beam epitaxy (MBE) and an anomalous HgCdTe alloy sample grown by liquid phase epitaxy (LPE). Convergence issues are also considered in that section. Some concluding comments regarding the suitability and practicality of implementing the QMSA technique as an industry standard are also provided.

MULTI-CARRIER SYSTEMS

The motion of carriers in a Hall sample may be described by the following set of Eq. (1)

$$J_{x} = \sigma_{xx}E_{x} + \sigma_{xy}E_{y}$$
$$J_{y} = \sigma_{yx}E_{x} + \sigma_{yy}E_{y}$$
(1)

where $\sigma_{xx} = \sigma_{yy}$ and $\sigma_{xy} = -\sigma_{yx}$ are the longitudinal and transverse conductivity tensor components, respectively, J_x and J_y are the current densities in the x and y directions, respectively, and E_x and E_y are the corresponding electric fields. The experimental Hall coefficient and resistivity are related to the components of the conductivity tensor through the following, relations:

$$R_{\rm H}(B) = \frac{\sigma_{xy} / B}{\sigma_{xx}^2 + \sigma_{xy}^2}$$

$$\rho(B) = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}$$
(2)

where B is the applied magnetic field in the z direction. For a sample involving more than one type of carrier, the conductivity tensor components can be expressed as a sum over the m species present within the multi-carrier system:

$$\sigma_{xx}(B) = \sum_{i=1}^{m} \frac{en_i \mu_i}{1 + (\mu_i B)^2}$$
$$\sigma_{xy}(B) = \sum_{i=1}^{m} S_i \frac{en_i \mu_i^2 B}{1 + (\mu_i B)^2}$$
(3)

where n_i and μ_i are the concentration and mobility of the i-th carrier species, respectively, and S_i is +1 for holes and -1 for electrons. It is primarily the $1+\mu^2B^2$ terms in the denominators of Eq. (3) which differentiate the contributions from the various carrier species. The contributions due to higher-mobility carriers (usually electrons) are the first to be "quenched" as B is increased; i.e., once μ B>>1 a given species exerts far less influence on $R_H(B)$ and $\rho(B)$. This phenomenon provides the field-dependent Hall data with its high degree of sensitivity to the individual mobilities.

MULTI-CARRIER FITTING PROCEDURE

The MCF is a procedure whereby Eq. (2) and Eq. (3) are employed to fit experimental data for $R_{\rm H}(B)$ and $\rho(B)$. In this method, $n_{\rm i}$ and $\mu_{\rm i}$ are the fitting parameters and the number of carriers, i, is typically between 2 and 5. The main drawback of the MCF is its arbitrariness. That is, not only must the many parameters in the model be optimized, but a decision needs to be made in advance with respect to what type and how many carriers to assume. The end result is that

the fit to the experimental Hall data is not unique.

MOBILITY SPECTRUM

Mobility Spectrum Analysis

The salient feature of the MSA developed by Beck and Anderson⁴ is that it transforms the experimental conductivity tensor vs magnetic field data into a continuous profile of the carrier mobilities present in the sample. The various electron and hole species then appear as peaks in the mobility spectrum. A major advantage of MSA over the MCF procedure is that it is inherently nonarbitrary; i.e., no prior assumptions are required. The derived spectrum may thus be viewed as simply a mathematical restatement of the original experimental Hall data.

The starting point for the MSA is to allow for the existence within the semiconductor sample of a continuous distribution of hole-like and electron-like carriers of any mobility. Equation (3) can thus be rewritten in integral form:⁴

$$\sigma_{xx}(B) = \int_{0}^{\infty} \frac{s^{p}(\mu) + s^{n}(\mu)}{1 + \mu^{2}B^{2}} d\mu$$
$$\sigma_{xy}(B) = \int_{0}^{\infty} \frac{\left[s^{p}(\mu) - s^{n}(\mu)\right]\mu B}{1 + \mu^{2}B^{2}} d\mu$$
(4)

where the hole and electron conductivity density functions (i.e., the mobility spectra) are given by

$$s^{p}(\mu) = ep(\mu)\mu$$

$$s^{n}(\mu) = en(\mu)\mu,$$
(5)

respectively, and $p(\mu)$ and $n(\mu)$ are the hole and electron concentration density functions, respectively. As stated earlier, the goal is to determine the conductivity density functions $s^{n}(\mu)$ and $s^{p}(\mu)$. However, the measured $\sigma_{xx}(B)$ and $\sigma_{xv}(B)$ do not uniquely define these density functions. Given values for the conductivity tensor at N different magnetic fields define a 2N-dimensional space which has, at most, 2N independent basis vectors. Since Eq. (4) defines an expansion of the data in terms of an infinite basis, the expansion cannot be unique. Using a rather complex mathematical formalism, Beck and Anderson were able to obtain unique envelopes $s^{n}(\mu)$ and $s^{p}(\mu)$ which represent physical δ -like amplitudes at μ . While this result may not be as valuable as finding unique functions $s^{n}(\mu)$ and $s^{p}(\mu)$, it is still very useful in that the various carrier species may at least be identified from the peaks in the envelope spectrum.

Dziuba and Gorska Iterative Approach

A different approach for obtaining the mobility spectrum was proposed by Dziuba and Gorska.⁵ Their more ambitious goal was to derive a quantitatively accurate mobility distribution instead of just an upper-bound envelope. In their approach, the integrals appearing in the conductivity tensor expression of Eq. (4) are approximated by sums of the partial contributions by carriers having a grid of discrete mobilities

$$\sigma_{xx} (B_{j}) = \sum_{i=1}^{m} \frac{\left[s^{p}(\mu_{i}) + s^{n}(\mu_{i}) \right] \Delta \mu_{i}}{1 + \mu_{i}^{2} B_{j}^{2}} = \sum_{i=1}^{m} \frac{S_{i}^{xx} \Delta \mu_{i}}{1 + \mu_{i}^{2} B_{j}^{2}}$$
$$\sigma_{xy} (B_{j}) = \sum_{i=1}^{m} \frac{\left[s^{p}(\mu_{i}) - s^{n}(\mu_{i}) \right] \mu_{i} B_{j} \Delta \mu_{i}}{1 + \mu_{i}^{2} B_{j}^{2}} = \sum_{i=1}^{m} \frac{S_{i}^{xy} \mu_{i} B_{j} \Delta \mu_{i}}{1 + \mu_{i}^{2} B_{j}^{2}} (6)$$

where S_i^{xx} and S_i^{xy} have elements defined as follows:

$$S_{i}^{xx} = s^{p}(\mu_{i}) + s^{n}(\mu_{i})$$
$$S_{i}^{xy} = s^{p}(\mu_{i}) - s^{n}(\mu_{i})$$
(7)

and the parameter m defines the number of points in the final mobility spectrum.

Using an initial spectrum (first trial function), which was obtained by a simpler approach than that of Beck and Anderson, Dziuba and Gorska were able to solve the set of Eqs. (6) using the Jacobi iterative procedure, in which the diagonal transformation matrix elements $1/(1+\mu_i^2 B_i^2)$ and $\mu_i B_i/(1+\mu_i^2 B_i^2)$ are simplified because of the specific choice of the mobility points $(\mu_i = 1/B_i)$ in the s^p (μ_i) and sⁿ (μ_i) spectra. Here, B_i is the i-th magnetic field obtained by spline interpolation of the experimental data in order to obtain the required density of points in the spectrum. Moreover, the diagonal elements are used as adjustable coefficients in the iteration process. An important consequence of this specific choice of mobility points is the fact that the mobility range in the spectrum is limited to $1/B_{max}^{exp} = \mu_{min} \le \mu \le \mu_{max} = 1/B_{min}^{exp}$, where B_{min}^{exp} and B_{max}^{exp} are the limits of the magnetic field in the experiment.

The goal of the procedure is to obtain the functional forms $s^p(\mu_i)$ and $s^n(\mu_i)$ which best fit the experimental magnetic field dependencies of σ_{xx} and σ_{xy} . "Nonphysical" results are allowed, since negative values of $s^p(\mu_i)$ and $s^n(\mu_i)$ are often obtained for some regions of the spectra.

Quantitative Mobility Spectrum Analysis

The QMSA approach presented in this paper is based on that of Dziuba and Gorska, with one key modification; that $s^{p}(\mu_{i})$ and $s^{n}(\mu_{i})$ are both constrained to be non-negative at all iteration steps. This is equivalent to requiring that no carriers can contribute negative conductivities. This step circumvents the ill-conditioning of Eq. (6), which can make the direct inversion of that equation meaningless. For definiteness, the MSA envelope (in discrete form) is used as the initial trial function, since the MSA spectrum is known to have approximately the correct overall shape. The final fit to experimental data tends to have lower error when the MSA is used as the first trial function rather than a simpler initial function. However, it is interesting to note that even a zeroedout initial function (i.e., $s^{p}(\mu_{i}) = s^{n}(\mu_{i}) = 0$) yields a reasonable final spectrum with only slightly higher error. In the present approach, the mobility range



Fig. 1. Normalized $(\sigma/\Delta\mu_i)$ mobility spectrum (QMSA) for InAs-GaSb single quantum well at 150K. Two carriers, an electron (E1) in the quantum well and a hole (H1) from the GaSb substrate can be identified.

considered by Dziuba and Gorska has been extended to values less than $1/B_{max}^{exp}$, which are often of considerable interest in semiconductor characterization, and represent values to which the data have a fairly high degree of sensitivity. A further improvement that has been implemented in the present procedure is in the efficiency with which the iterative solution is obtained in comparison to that employed by Dziuba and Gorska. To solve for S^{xx} and S^{xy}, we first rearrange Eq. (6):

$$S_{i}^{xx} = \left(1 + \mu_{i}^{2}B_{i}^{2}\right) \left[\sigma_{xx}^{exp}(B_{i}) - \sum_{j\neq i}^{m} \frac{S_{j}^{xx}}{1 + \mu_{j}^{2}B_{i}^{2}}\right]$$
$$S_{i}^{xy} = \frac{\left(1 + \mu_{i}^{2}B_{i}^{2}\right)}{\mu_{i}B_{i}} \left[\sigma_{xy}^{exp}(B_{i}) - \sum_{j\neq i}^{m} \frac{S_{j}^{xy}\mu_{j}B_{i}}{1 + \mu_{j}^{2}B_{i}^{2}}\right]$$
(8)

If the values of S_i^{xx} and S_i^{xy} from the previous iteration are substituted into the right-hand side of Eq. (8), and if their new values are used as soon as they become available, the new set of values $S_i^{xx}(k+1)$ and $S_i^{xy}(k+1)$ can be determined from the following Gauss-Seidel iterative procedure

$$\begin{split} S_{i}^{xx}(k+1) = \\ & \left(1 + \mu_{i}^{2}B_{i}^{2}\right) \left[\sigma_{xx}^{exp}(B_{i}) - \sum_{j=i}^{i-1} \frac{S_{j}^{xx}(k+1)}{1 + \mu_{j}^{2}B_{i}^{2}} - \sum_{j=i+1}^{m} \frac{S_{j}^{xx}(k)}{1 + \mu_{j}^{2}B_{i}^{2}}\right] \end{split}$$



a

Fig. 2. (a) Carrier density and (b) mobility as a function of temperature for the InAs-GaSb single quantum well obtained from QMSA (see Fig. 1); an electron (E1) in the quantum well and a hole (H1) from the GaSb substrate are evident.

$$S_{i}^{xy}(\mathbf{k}+1) = \frac{(1+\mu_{i}^{2}B_{i}^{2})}{\mu_{i}B_{i}}$$
$$\left[\sigma_{xy}^{exp}(B_{i}) - \sum_{j=1}^{i-1} \frac{S_{j}^{xy}(\mathbf{k}+1)\mu_{j}B_{i}}{1+\mu_{j}^{2}B_{i}^{2}} - \sum_{j=i+1}^{m} \frac{S_{j}^{xy}(\mathbf{k})\mu_{j}B_{i}}{1+\mu_{j}^{2}B_{i}^{2}}\right]$$
(9)

If $S_i^{xx}(k)$ and $S_i^{xy}(k)$ are added and subtracted, respectively, from the right-hand side of the corresponding expressions in Eq. (9), and if the constant ω is introduced such that

$$S_{i}^{xx}(\mathbf{k}+1) \approx (1-\omega)S_{i}^{xx}(\mathbf{k}) + \omega$$

$$\left\{ \left(1+\mu_{i}^{2}B_{i}^{2}\right) \left[\sigma_{xx}^{exp}(\mathbf{B}_{i}) - \sum_{j=1}^{i-1} \frac{S_{j}^{xx}(\mathbf{k}+1)}{1+\mu_{j}^{2}B_{i}^{2}} - \sum_{j=i+1}^{m} \frac{S_{j}^{xx}(\mathbf{k})}{1+\mu_{j}^{2}B_{i}^{2}} \right] - S_{i}^{xx}(\mathbf{k}) \right\}$$

$$S_{i}^{xy}(\mathbf{k}+1) = (1-\omega)S_{i}^{xy}(\mathbf{k}) + \omega \qquad (10)$$

$$\left\{\!(\frac{1\!+\!\mu_i^2 B_i^2}{\mu_i B_i}\!)\!\left[\sigma_{xy}^{exp}\!\left(B_i\right)\!-\!\sum_{j=1}^{i-1}\!\frac{S_j^{xy}\!\left(k\!+\!1\right)}{1\!+\!\mu_j^2 B_i^2}\!-\!\sum_{j=i+1}^m\!\frac{S_j^{xy}\!\left(k\right)}{1\!+\!\mu_j^2 B_i^2}\right]\!-\!S_i^{xy}\!\left(k\right)\!\right\}$$

then the successive over-relaxation iteration algorithm is obtained in which the coefficient ω controls the convergence speed of the procedure. Although this algorithm is not guaranteed to converge, convergence has in fact been obtained for every one of the many experimental data sets analyzed so far. In the standard iteration procedure (in which $\omega = 1$), the mobility spectrum is modified so rapidly that even after the first iteration step the qualitative information contained in the shape of the envelope spectrum is destroyed.

To ensure that such information is preserved, a value of $\omega = 0.01$ was chosen in our calculations so that modification of the mobility spectrum was slowed down in the successive iterations. In order to obtain more accurate results, interpolation between the experimental points for $\sigma_{xx}(B)$ and $\sigma_{xy}(B)$ has been carried out using a spline technique, resulting in a density of 50 points per decade. This allows the spectrum to be derived with much higher resolution in comparison to that obtained by Dziuba and Gorska who used only ten points per decade.

It is important to note that the amplitudes of $s^{p}(\mu_{i})$ and $s^{n}(\mu_{i})$ in the QMSA depend on the density of points used for the calculation. Thus, in order to obtain the total conductivity corresponding to the carrier represented by a particular peak, all the amplitudes under that peak must be added together.

RESULTS AND DISCUSSION

It was remarked in the introduction that the QMSA can be applied to any magnetic-field-dependent Hall and resistivity data (as long as the concentrations and mobilities do not depend on magnetic field and quantum oscillations are not prominent). In this section, we present representative results illustrating the analysis for two dissimilar semiconductor systems: an InAs-GaSb single quantum well whose relatively simple mobility spectrum displays only one electron peak and one hole peak, and an LPE-grown HgCdTe (x = 0.216) alloy sample whose more complex spectra will be discussed in more detail.

InAs-GaSb Single Quantum Well

As a first example, we consider results for a GaSb-InAs-GaSb single quantum well with thickness 200Å. Figure 1 presents the QMSA mobility spectrum for the quantum well at T = 150K. The spectrum is seen to display sharply resolved peaks corresponding to one electron species (the two-dimensional electron



b

Fig. 3. (a) Mobility spectrum (QMSA) at 80 and 110K, and Beck and Anderson (B&A) envelope at 110K; and (b) experimental (points) and calculated (curves) using QMSA of the conductivity tensor components at 110K for LPE HgCdTe (x = 0.216).



Fig. 4. Convergence in the QMSA iterative procedure according to Eq. (11) for (a) σ_{xx} and (b) σ_{xy} for LPE HgCdTe (x = 0.216) at three temperatures: 70, 110, and 150K.

residing in the quantum well, labeled E1) and one hole species (the three-dimensional, bulk, majority carrier in the GaSb substrate, labeled H1). As was mentioned in the section on QMSA, the magnitude of the conductivity contributions creating the QMSA spectrum depends on the density of points in such a way that the total conductivity remains constant. In order to present the results in a form which does not depend on the mobility increment chosen, the spectrum in Fig. 1 has been normalized by dividing the partial conductivity contributions by the mobility increment (i.e., $\sigma_i / \Delta \mu_i$). The net carrier density for a given species can also be obtained, by summing over the incremental contributions under the peak corresponding to that carrier:

$$n = \sum \sigma_i / (e\mu_i).$$

Temperature-dependent carrier densities and mobilities for both E1 and H1 were determined from the QMSA spectra at a series of temperatures between 30 and 300K, and are shown in Fig. 2. Note that H1 freezes out in the low-temperature limit. The mobility and concentration results derived from the QMSA procedure are quite similar to those obtained from a conventional MCF fit. The significant difference, however, is that the QMSA spectra were obtained from a fully automated algorithm, whereas the MCF required initial assumptions about the number and types of carrier species to employ in the fitting procedure.

LPE HgCdTe Sample

The second data set to be considered are for an LPEgrown HgCdTe alloy (x = 0.216) film provided by Loral. The electrical properties of this sample were anomalous, which probably accounts for the complexity of its mobility spectra. Typical QMSA results for this sample are presented in Fig. 3a, which illustrates the electron spectra for T = 80 and 110K (the hole conductivities are much smaller, so we will ignore them in this discussion). Note that the 80K spectrum displays two sharp peaks (E1 and E2), while the 110K spectrum contains two peaks (E1 and E3) plus a broad shoulder where E2 had been (the identification of these three species will be discussed below). The solid line indicated as B&A is the initial, discrete form, of the Beck and Anderson envelope for the iterative procedure. For the 110K data, Fig. 3b demonstrates that the final QMSA fits (curves) to the experimental (points) conductivity tensor components σ_{xx} and σ_{xy} are almost perfect. Although the QMSA mobility spectrum changes dramatically during the iterative procedure, it still preserves the qualitative features of the Beck and Anderson MSA envelope that was used as the initial trial function. However, whereas the MSA spectrum provides only qualitative information, the final QMSA spectrum also yields an accurate quantitative determination of the mobility and density of each electron species.

Figure 4 shows the convergence process for the spectra obtained at temperatures of 70, 110, and

150K. The convergence is measured as an error, defined in the same way for both conductivity tensor components σ_{xx} and σ_{xy} :

$$\Delta \mathbf{E}^{2}(\mathbf{k}) = \frac{\sum_{i} \left[\sigma_{i}^{exp} - \sigma_{i}^{QMSA}(\mathbf{k})\right]^{2}}{\sum_{i} \left[\sigma_{i}^{exp}\right]^{2}}$$
(11)

where σ_i^{exp} and σ_i^{QMSA} are the experimental and QMSA values, respectively, and k is the iteration step number. For most of the samples analyzed so far, the error $\Delta E(k)$ decreases to its minimum value (best fit) after approximately 50 iterations (with $\omega = 0.01$). A characteristic feature of the error is that it is smaller for the σ_{xx} component (about 1%) than for σ_{xy} component (about 2–4%). This is probably because the experimental data for σ_{xx} are more accurate than those for σ_{xy} (at low magnetic fields, the Hall voltage is an order of magnitude less than the resistivity voltage).

Quantitative mobility-spectrum analysis of the magneto-transport data taken at a number of different temperatures between 4.2 and 300K was used to extract temperature-dependent carrier concentrations and mobilities (see Fig. 5a and 5b, respectively) for all three of the carrier species. Note that whereas both n and μ for E1 and E2 are nearly independent of T, the density for the higher-mobility species E3 increases rapidly with increasing temperature. This is clearly the intrinsically generated electron which occupies the bulk of the HgCdTe epitaxial layer. The two lowermobility species E1 and E2 therefore reside somewhere else, perhaps at the surface or in the gradedgap buffer region between the CdTe substrate and the HgCdTe film. As such, their carrier concentrations should more properly be represented as sheet densities, which are found to be 5.10¹¹cm⁻² for E1 and $2 \cdot 10^{11} \text{cm}^{-2}$ for E2. Since the E3 species is so dominant that its peak completely obscures the other two at temperatures above 150K, densities and mobilities for E1 and E2 are not shown in Fig. 5 for temperatures in that range.

For comparison purposes, the same data sets were also analyzed by the standard multi-carrier fitting procedure, using the Marquardt-Levenberg nonlinear least-squares curve-fitting algorithm implemented in the MicroCal Origin[™] software package. Although the error in fitting the conductivity tensor was relatively small for any MCF calculation employing three or more species, the qualitative behavior of the resulting densities and mobilities was highly dependent on how many carriers were assumed to be present. Assuming three species, for example, at low temperature two of them obviously corresponded to E1 and E2 from Fig. 3a, while the third had a much lower mobility. However, at temperatures above 100K, the highest-mobility species increased its mobility (corresponding to E3) while the intermediate-mobility species appeared to become a composite of E1 and E2. When four species were assumed, the mix became even more complicated, dramatically illustrating the

extreme sensitivity of the MCF to the arbitrary initial assumption concerning species multiplicity. Thus, there is considerable advantage to the elimination of prior assumptions in the QMSA, even though it is not always a straightforward matter to interpret the



b

Fig. 5. (a) Carrier density and (b) carrier mobility as a function of temperature for LPE HgCdTe (x = 0.216) obtained from the mobility spectrum (QMSA). Three identified carriers indicated as E1, E2, E3.

identity of the various peaks and shoulders which appear in the spectra. In contrast to the standard MCF, the data manipulation phase of the QMSA magneto-transport characterization is clearly differentiated from the interpretation phase.

CONCLUSIONS

We have discussed a new approach to obtaining quantitative mobility and carrier density information from the analysis of field-dependent Hall and resistivity data. Starting with an appropriate initial trial function such as the Beck and Anderson spectrum (in discrete form), the iterative algorithm of the QMSA generates electron and hole mobility spectra which yield almost perfect fits to the experimental conductivity tensor as a function of magnetic field. The spectra obtained may be viewed as an easily interpreted graphical restatement of the input data. It fully quantifies the number of carrier species (from the number of peaks), their type (electrons or holes), and their densities and mobilities. While the QMSA results are often similar to those obtained from a standard multi-carrier fit, the procedure is fully automatic and does not require any initial assumptions.

In most regards, the iterative approach presented in this paper does not differ appreciably from that of Dziuba and Gorska. We have employed a more realistic initial function (the MSA mobility spectrum), significantly increased the density of points in the spectrum, extended the mobility limits, and employed a more efficient iteration algorithm (the successive overrelaxation procedure). In practice, however, the most significant difference is that the convergance has been improved by constraining the partial conductivity contributions to always have non-negative values (which is also more physically reasonable). These refinements have made the technique more practical and reliable to use.

For a PC with a 486 processor, the total CPU time needed to generate the QMSA spectrum for a single

temperature (including experimental data interpolation, the MSA spectrum calculation, and the QMSA itself) is in the order of 2 min. Presently, the only step requiring human intervention is in the determination of carrier densities corresponding to a given mobility peak, since one must choose the range of mobilities to be integrated over for each peak. Ultimately, however, this step could also be automated in more routine cases where the general nature of the spectrum is somewhat known in advance.

Further refinements of the QMSA technique are now under investigation. Also being initiated is a detailed study of how the QMSA performs when it is routinely applied to a large number of samples with widely varying properties. However, preliminary indications suggest that the present form of the procedure is quite suitable for use as an industry-standard tool for analyzing field-dependent Hall characterizations of diverse semiconductor materials and bandgap engineered structures.

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