Chapter 3

A review of mobility spectrum analysis

3.1 Introduction

In this chapter, many variant techniques for the mobility spectrum calculation are described. We will start with a discussion on the characteristic of mobility spectrum problem. Then the existing techniques comprised of the procedure purposed by Beck and Anderson (1987), an iterative technique by Dziuba and Gorska (1992), a Quantitative Mobility Spectrum Analysis (QMSA) by Antoszewski et al. (1995), an improved Quantitative Mobility Spectrum Analysis (i-QMSA) by Vurgaftman et al. (1998), and a Maximum Entropy Mobility Spectrum Analysis (ME-MSA) by Kiatgamolchai et al. (2002*a*) will be reviewed briefly.

3.1.1 Inverse problem

The mobility spectrum problem is to determine $s(\mu)$ by solving the conductivity equations (Eqs. (2.25) and (2.26)) which have the form of the Fredholm integral of the first kind. The Fredholm integral of the first kind takes a general form of [Press et al. (1992)]

$$g(t) = \int_a^b K(t,s)\, f(s)\, ds. \tag{3.1}$$

The left-hand-side term $g(t)$ is a known quantity. $f(s)$ is an unknown function and $K(t,s)$ is the kernel function of two variables. If the variables t and s are discrete, Eq. (3.1) can be expressed in a matrix form

$$\mathbf{g} = \mathbf{K} \cdot \mathbf{f}. \tag{3.2}$$

Eq. (3.2) can be solved easily by inverting the kernel matrix if it is not singular. In general, the Fredholm integral is so ill-conditioned that the kernel matrix is nearly singular or its condition number is very large. The solution is therefore extremely sensitive to a small change or error in data. This kind of the problem is known as the inverse problem. Solving the inverse problem cannot be done directly in this manner. Examples of inverse problem are a deconvolution problem, an image and spectrum reconstruction, and some spectral analysis problems including the mobility spectrum.

3.1.2 Mobility spectrum problem

By comparing Eqs. (2.25) and (2.26) to Eq. (3.1), the known functions are the conductivity tensor components $\sigma_{xx}(B)$ and $\sigma_{xy}(B)$. The conductivity density $s(\mu)$ is the unknown function to be solved for and the kernels are

$$K_{xx}(\mu, B) = \frac{1}{1 + (\mu B)^2} \tag{3.3}$$

and

$$K_{xy}(\mu, B) = \frac{\mu B}{1 + (\mu B)^2}. \tag{3.4}$$

The plot of kernels versus μB are shown in Fig. 3.1. The kernel is strongest dependent on μB at $\mu B = 1$ [Dziuba and Gorska (1992)] which is called unity condition. By this condition, it is suggested that the lowest mobility $(m^2V^{-1}s^{-1})$ which can be resolved effectively is about $B^{-1}\,(T^{-1})$.

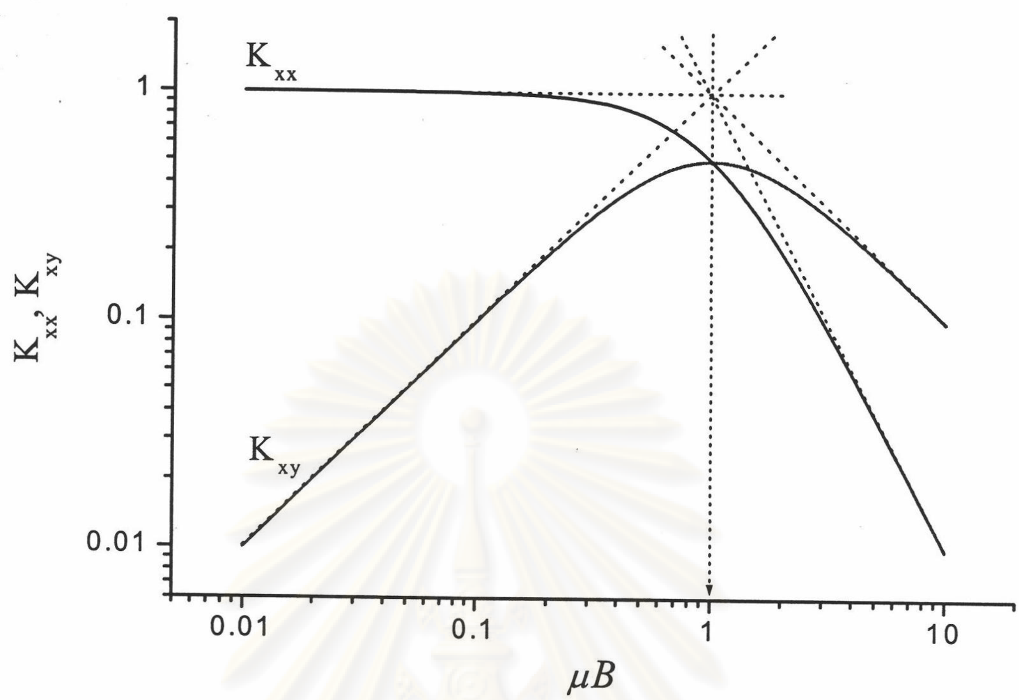

Figure 3.1: The kernel functions of magnetoconductivity $\sigma_{xx}(B)$ and $\sigma_{xy}(B)$ (after Kiatgamolchai (2000)).

3.2 Beck and Anderson mobility spectrum

A mobility spectrum analysis was developed by Beck and Anderson (1987) for a multi-carrier characterization. The method employed the magnetic-field-dependent resistivity $\rho_{xx}(B)$ and Hall coefficient $R_H(B)$ obtained from experiments. From McClure's expression for the magnetic-field-dependent conductivity, Beck and Anderson derived a relation between the magnetoconductivity tensor components $\sigma_{xx}(B)$, $\sigma_{xy}(B)$, and the conductivity density $s(\mu)$ under the influence of magnetic field via the integral equations (Eqs. (2.25) and (2.26)) which have been discussed in Section 2.2. They suggested that the determination of mobility spectrum $s(\mu)$ provides all fundamental information of the electrical transport; for example,

1) The conduction in multiple bands with different mobilities are represented as distinct peaks in $s(\mu)$.

2) The broadening of a peak in $s(\mu)$ corresponds to an energy-dependent relaxation time (τ) in a given band with the Hall factor $r_H = \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2}$ and a distribution of relaxation time can be determined. The presence of a non-parabolic band at finite temperatures also broadens the peak.

3) The non-spherical Fermi surface for a given band causes harmonic peaks in $s(\mu)$.

Basically, the feature of mobility spectrum analysis is to extract the number of carrier species with their mobilities and carrier concentrations. To do this, the conductivity tensor components are measured at a finite number of magnetic field points, but $s(\mu)$ is quasi-continuous in mobility space. It means that there is not enough data to define $s(\mu)$ uniquely.

However, Beck and Anderson have developed a mathematical procedure to determine a unique envelope of all $s(\mu)$ that corresponds to a given set of data. Firstly, the procedure performs a physical test to check a validity of measured data. In physical test stage, measured data will be grouped into a combinatorial subset of a few data points, and eigenvalues of the matrix associated with data are calculated. For any subset to be *physical*, their corresponding eigenvalues must be nonnegative. Then the nonnegative eigenvalues and their eigenfunctions are used to calculate $s(\mu)$, and the unique envelope of all $s(\mu)$ is obtained. In practical, the procedure requires the assumption of number of carrier species. Moreover, the number of data in each subset should be at least $N+1$ points since N is a number of carrier species in the sample. In fact, increasing a number of data points per subset leads to the extreme decrease of passing rate of the physical test. The number of acceptable $s(\mu)$ is also decreased. When this happens, the envelope becomes unreasonable and does not represent the carrier correctly.

In summary, this technique is a qualitative method to calculate the envelope of mobility spectrum. It has been demonstrated with synthetic data and experimental data of HgCdTe and GaAs/AlGaAs heterostructures.

3.3 Quantitative method

Dzuiba and Gorska (1992) approximated the integral transforms (Eqs. (2.25) and (2.26)) into the discrete forms as

$$\sigma_{xx}(B_j) = \sum_{i=1}^{N} \frac{s_i^{xx}}{1+\mu_i^2 B_j^2} \tag{3.5}$$

and

$$\sigma_{xy}(B_j) = \sum_{i=1}^{N} \frac{s_i^{xy}\mu_i B_j}{1+\mu_i^2 B_j^2}, \tag{3.6}$$

where the partial conductivities s_i^{xx} and s_i^{xy} contain both hole and electron partial conductivities s^p and s^n as

$$s_i^{xx} = s_i^p + s_i^n \tag{3.7}$$

and

$$s_i^{xy} = s_i^p - s_i^n. \tag{3.8}$$

N is the number of mobility mesh points which are defined within our interested mobility range of mobility spectrum. The partial conductivity of index i is associated with the mobility μ_i, and the problem becomes linear in mobility space.

For the system of linear Eqs. (3.5) and (3.6), the number of mobility points N is set equal to the number of magnetic field points. The mobility value is selected with the condition $\mu_i B_i = 1$. As a result, the mobility range is limited to $\mu_{\min} = B_{\max}^{-1}$ and $\mu_{\max} = B_{\min}^{-1}$ where B_{max} and B_{min} are the maximum and minimum magnetic field strength.

Dziuba and Gorska solved the system of Eqs. (3.5) and (3.6) by using the Jacobi iteration procedure (see Gerald et al. (1986)). The iterative part is expressed as

$$s_{i,k}^{xx} = s_{i,k-1}^{xx} + \left(\sigma_{xx}^{\exp}(B_i) - \sigma_{xx}(B_i)\right)\alpha_{xx} \tag{3.9}$$

and

$$s_{i,k}^{xy} = s_{i,k-1}^{xy} + \left(\frac{\sigma_{xy}^{\exp}(B_i) - \sigma_{xy}(B_i)}{B_i}\right)\alpha_{xy}, \tag{3.10}$$

where k is the number of iterations. The parameter α_{xx} and α_{xy} (usually less than 1) are adjustable to stabilize the convergence. In this technique, the mobility spectrum was found to show dominant peaks situated at the mobility of each carrier species but with oscillation of partial conductivity around the zero level. The oscillation occurred as the feature of smoothness due to the algorithm. It causes a negative conductivity at some mobility value and is considered unphysical. Dzuiba and Gorska summarized that the quality of the mobility spectrum from this numerical technique is limited by the range of the magnetic field, the number of data points, a finite number of iterations and experimental errors.

Antoszewski et al. (1995) modified the iterative technique and named it Quantitative Mobility Spectrum Analysis (QMSA). It was extended to an improved-Quantitative Mobility Spectrum (i-QMSA) later [Vurgaftman et al. (1998)]. QMSA used Gauss-Seidel successive over-relaxation iteration (see Gerald et al. (1986)) to improve the convergence speed. Iterative parts are

$$s_{i,k}^{xx} = (1-\omega_{xx})\, s_{i,k-1}^{xx} + \omega_{xx}\left(1+\mu_i^2 B_i^2\right)\left[\sigma_{xx}^{\exp}(B_i) - \sum_{j=1}^{i-1}\frac{s_{j,k}^{xx}}{1+\mu_j^2 B_i^2} - \sum_{j=i}^{N}\frac{s_{j,k-1}^{xx}}{1+\mu_j^2 B_i^2}\right] \tag{3.11}$$

and

$$s_{i,k}^{xy} = (1-\omega_{xy})\, s_{i,k-1}^{xy} + \omega_{xy}\frac{\left(1+\mu_i^2 B_i^2\right)}{\mu_i B_i}\left[\sigma_{xy}^{\exp}(B_i) - \sum_{j=1}^{i-1}\frac{s_{j,k}^{xy}\mu_j B_i}{1+\mu_j^2 B_i^2} - \sum_{j=i}^{N}\frac{s_{j,k-1}^{xy}\mu_j B_i}{1+\mu_j^2 B_i^2}\right], \tag{3.12}$$

where ω_{xx} and ω_{xy} are parameters adjustable to control the convergence speed. The mobility range is extended to cover the mobility lower than $B_{\max}^{-1}$ by an extrapolation of the measured data beyond the maximum magnetic field strength. The density of mobility points in spectrum is also increased by data interpolation between the adjacent experimental data using a spline technique. In order to avoid an unphysical interpretation, the partial conductivities are constrained to be nonnegative during the iteration processes. They suggested that Beck and Anderson mobility spectrum can be used as an appropriate initial trial spectrum for QMSA.

In i-QMSA, the condition $\mu_i B_i = 1$ is elevated. The number of mobility points and their values are arbitrarily chosen, independent of the number of magnetic fields and their strength. Especially, the number of mobility points can be larger than the number of magnetic fields. In order to yield a good fit, this technique employs many data manipulations, such as first derivative fitting, two/three-point swapping and point elimination. The result is smoother than those from previous calculations, and also physical.

These iterative procedures have been developed for a commercial use, and it was tested over a variety of samples, such as HgTe and HgCdTe. The only drawback is their data manipulation techniques and other individual bias which may deviate the spectrum from uniqueness and true interpretation.

3.4 Maximum entropy mobility spectrum analysis

The maximum entropy principle was first applied to the mobility spectrum analysis by Kiatgamolchai et al. (2002*a*) and later named Maximum Entropy Mobility Spectrum Analysis (ME-MSA). Using the information concept of the entropy, a unique solution is extracted from a limited number of data.

The entropy function H of the probability distribution $\{p_i | i = 1, 2, ..., N\}$ is defined in a unique way as [Jaynes (1957)]

$$H\{p_i\} = -\sum_{i=1}^{N} p_i \ln p_i, \tag{3.13}$$

where $\sum_i p_i = 1$ and $p_i \geq 0$ for all i.

The set of partial conductivity $\{s_i | i = 1, 2, ..., N\} = \{s_1^p, s_2^p, ..., s_{\frac{N}{2}}^p, s_{\frac{N}{2}+1}^n, s_{\frac{N}{2}+2}^n, ..., s_N^n\}$ (see Section 3.3) is related to a probability distribution $\{p_i\}$ by

$$p_i = \frac{s_i}{\sigma_0}, \tag{3.14}$$

where σ_0 is the conductivity at zero magnetic field. s_i is simply equal to $n_i e \mu_i$. By the concept of probability, the partial conductivities are forced to be positive automatically. The principle of this procedure is to maximize the entropy Eq. (3.13) of the normalized spectrum Eq. (3.14) subjected to the system of Eqs. (3.5) and (3.6) as constraints. The Lagrange multiplier method is used to express the solution of this problem [Jaynes (1957)]. Kiatgamolchai et al. (2002*a*) determined the unknown Lagrange multipliers to obtain the maximum-entropy mobility spectrum by applying a formalism from Agmon et al. (1979) and an iterative technique from Hollis et al. (1992).

In this approach, the condition $\mu_i B_i = 1$ is not necessary. The number of mobility points can be selected to be greater than the number of data points. Also the mobility range is not constrained by the magnetic field strength. The inter/extrapolation of data and the empirical manipulation procedure is not required. For a given data set, a unique and physically reasonable mobility spectrum is obtained. The resultant spectrum shows high degree of smoothness with a good fit to data. It overcame the previous procedure in such that it is less sensitive to measurement errors, and the low-mobility carrier species can be observed easier. More details of entropy and information theory are discussed in Section 4.2.

3.5 Summary

The inverse problem of mobility spectrum calculation has been solved by different techniques. The later developed procedure has overcome the previous procedure. The difficulties of the problem such as the sensitivity to error and the recovering or low carrier species are improved. However, an error analysis is not involved in those reviewed techniques.