Chapter 6

Conclusions and suggestions

In this thesis, a mobility spectrum analysis is concerned. We have developed a new mobility spectrum calculation based on Bayesian statistics and the maximum entropy principle, called the Bayesian method. The crucial feature of this new technique is an error analysis that allows the uncertainty estimation of the calculated results. The program is tested under varying conditions on a personal computer Pentiam 4, 1.7 GHz. The computing time is about 4 minute per 1 million iterations (sampling) for a matrix size of 50×200, a number of mobility points (50) and twice a number of magnetic points (100) respectively. The advantages of the developed technique can be summarized as follow.

1. The pre-assumption about a number of carrier species, as parameters, is not necessary in contrast to a general fitting method.

2. The number of mobility points in spectrum can be selected independent to the number of magnetic field points. In addition, all of data points can be used without considering the linearly independent of the data set. This is because the algorithm is based on the random process, not a matrix manipulation.

3. Harmonic peaks are not observed.

4. By using Bayes' theorem, the model of mobility spectrum problem can be extended to nonlinear model if the further development is required.

5. The calculation provides an uncertainty in solution that helps estimate a degree of confidence in the results. One can calculate the error bars for mobility, carrier concentration and carrier conductivity. The error bar is also useful to infer the artifact peak whose error bar is large compared to its conductivity.

It is found that the magnitude of conductivity uncertainty depends on many factors which are experimental noise, a number of data points, a value of standard deviation in the likelihood distribution, a maximum magnetic field (μB condition), and the conductivity ratio between the carrier species. The major factor is experimental noise. It is noted that only random noise is considered in the thesis because it can be studied easily using a statistical model. Noise not only increases the uncertainty in the solution but also contributes to a poor spectrum such as presenting a very broad peak and splitting peak. Empirically, the computer program is well operating if noise level do not exceed 0.5%. The number of data points influences the solution when it is less than the number of mobility points. From the results, however, it cannot be concluded that this condition is well acceptable since the ratio of data points to mobility points is greater than unity. Increasing the number of mobility points also leads to the same result. The standard deviation in chi-square, which is a defined width of a likelihood distribution, affects the uncertainty in the solution where noise is not presented in the data. It is not clear to conclude which factors between noise and standard deviation are dominant because they cannot be treated independently. The maximum strength of magnetic field also influence the result. It is found that if a lowest-mobility carrier species satisfies the condition $\mu B < 1$, the solution will be reported with high level of uncertainty. The uncertainty distributes to each carrier species with different magnitudes according to the conductivity percentage of each carrier species.

The temperature-dependent electrical property of a modulation-doped p-type $Ge/Si_{0.4}Ge_{0.6}$ heterostructure in temperature range 200-300 K has been studied using the Bayesian method and maximum-entropy mobility spectrum analysis. The mobility spectra obtained from two calculation techniques are well consistent. Both spectra presents two major hole carrier species and an electron-like carrier species. Only two hole species are interested because their sources are already known according to the material design. A high mobility carrier is the two-dimensional hole gas in a Ge quantum well. As the temperature increases form 200-300 K, the mobility and carrier concentration of 2DHG monotonically decreases from 4,700 to 2,500 $cm^2V^{-1}s^{-1}$ and from 1.7×10^{12} to 1.3×10^{12} cm^{-2}, respectively. A lower mobility carrier species is the boron-doped layer ($B:Si_{0.4}Ge_{0.6}$). The B:SiGe peak slightly shifts to the low mobility and gains the conductivity as the temperature increases. At room temperatures, the doped species has the mobility of 800 $cm^2V^{-1}s^{-1}$ and concentration of 1.48×10^{12} cm^{-2}. Even though its mobility is too high compared to the existing experimental reports on boron-doped mobility at lower Ge ratio, the result is similar to that of Kiatgamolchai (2000).

For further development of the Bayesian method, there are many topics need the improvement:

1. If a number of mobility points is large (≥ 50) the calculation fails because of an extra-low acceptance rate.
2. Many parameters in the computer program are empirically tested by trial and error; for examples,
   (a) α tuning : the selecting of stopped alpha may be subjected to human bias.
   (b) A number of iterations per α step : there is no procedure to monitor the convergence of a Markov chain.

To overcome these problems, we suggest to improve the Markov chain generator in order to yield a sufficient acceptance rate with rapid convergence rate. The used generator in this thesis is a basic algorithm that suitable for educational examples, and there are many modified algorithms that well suit for the specific problem. The procedure should be extended from a one-chain process to a multiple-chain process so that the convergence can be monitored from the merging of all Markov chains. To do this, the efficiency of chain generator and calculation machine is required. The last point, if the probability of the mobility spectrum at each stopped α can be evaluated, the stopped α that gives the most probability should be selected. Alternatively, if there are many stopped α's that are probably significant, a weight mean of all probable spectrum can be represented as the best solution.