Using Neural Networks for RHEED Modeling of Interfaces in AlGaSb-InAs HEMT Devices

Gregory E. Triplett, Gary S. May, and April S. Brown

School of Electrical & Computer Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0250
triplett@ece.gatech.edu - (404) 894-9904, gary.may@ee.gatech.edu - (404) 894-9420, april.brown@ee.gatech.edu - (404) 894-5161

Abstract

In this paper, it is demonstrated that RHEED data obtained during the formation of the interfaces in AlGaSb-InAs HEMT devices can be used to model device important epitaxial layer electrical performance parameters. RHEED intensity oscillations of the specular spot are analyzed using principle component analysis (PCA) and modeled using error back-propagation (BP) neural networks.

INTRODUCTION

Compound semiconductor electronic devices have been produced by molecular beam epitaxy (MBE) with excellent performance at high frequencies. However, barriers to reproducible and high performance devices exist when growing structures with mixed anion interfaces. Reasons for this are not yet well understood and are related to growth processes and structural properties. Reflection high-energy electron diffraction (RHEED) provides information about the growth dynamics and atomic arrangements of the growth surface in real-time. In this paper, RHEED is used to investigate one particular barrier, interface formation, which is critical for future manufacturing efforts. We will use the AlGaSb-InAs high electron mobility transistor (HEMT) as the device demonstration for our efforts. This HEMT technology is the next generation for high speed and millimeter wave electronics. Interface quality is key to achieving high electron mobility and velocity in these structures.

As/Sb interfaces are known to be affected by anion intermixing and exchange [1, 2]. Ultimately, the performance of As/Sb heterojunction devices by MBE is dependent on the exact growth conditions employed at the interfaces. RHEED is particularly promising in this regard because real time analysis at the atomic level may provide an understanding of the growth processes present at the As/Sb mixed interface, as well as present a potential opportunity to adjust the growth conditions during production. It has been demonstrated that RHEED can be used to observe anion exchange reactions [3]. RHEED also provides information about the roughness of the growing surface. Since carrier transport is sensitive to interfacial roughness (impurity scattering), RHEED can be correlated to electron-mobility. This paper demonstrates that information about the quality of the As/Sb mixed interface is present in the RHEED data, and this data can be used to model device performance parameters. Neural networks are used to develop the models described in this paper.

EXPERIMENTAL TECHNIQUE

Experiments were performed in a Varian Gen-II MBE system. The test vehicle in this study was an InAs-$Al_{0.66}Ga_{0.33}Sb$ HEMT structure developed in previous experiments. The HEMT structure is shown in Figure 1. The structure from cap layer to substrate consists of the following: 3-nm GaSb / 17-nm AlSb / 15-nm InAs / 200-nm $Al_{0.66}Ga_{0.33}Sb$ / (5-nm AlSb / 5-nm GaSb) X15 / 2-µm AlSb / 300-nm GaSb / 200-nm GaAs buffer / GaAs substrate.

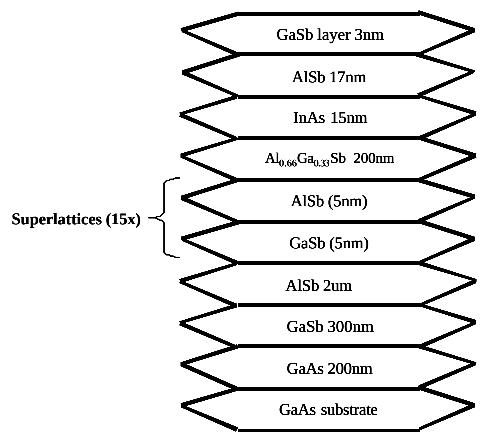


Figure 1. InAs-AlGaSb based HEMT test Structure

The HEMT structures were grown on one-quarter of 2"-GaAs (100) undoped substrates. Samples were mounted in indium-less *EPI* substrate assemblies. Experiments were performed under Group-V stabilized conditions, where the growth rates for In, Ga, and Al were 0.5, 1.0, and 2.0 µm/hr, respectively. Arsenic tetramers (As_4) and antimony dimers/monomers (Sb_2/Sb) were used in these experiments. All samples were rotated during growth, except when RHEED oscillations were recorded during the formation of the interface. The growth temperatures were determined using the deoxidation temperature of GaAs substrates (~580°C).

The experiments focus on the formation of the inverted interface, InAs-on-AlGaSb. At this interface, a twenty-second Sb soak, followed by indium deposition preceded InAs channel growth. The Sb soak was used to saturate the surface sites with Sb atoms, so that an InSb-like bonding configuration could be formed.

EXPERIMENTAL DESIGN

Since the conversion of the inverted interface into InSb-like bonds is required for high electron mobility, the growth conditions before and during the growth of the InAs channel are critical [4]. Typically, Sb soaks or deposition of one indium monolayer are used to form the InSb-like bonds. Previous work [2] describes the amount of indium necessary to create a smooth InAs/AlSb interface. This report suggests that more than one indium monolayer is required to make up for the compositional difference in the two reconstructions. In an attempt to illuminate indium's impact on the bond configuration of the interface, channel growth temperature and indium barrier thickness at the interface are varied. A statistically designed experiment is used to perform the experiments. This design is a 2^2 full-factorial central composite circumscribed (CCC) experiment requiring eleven runs [5]. Table 1 shows the factors, ranges and units of the parameters studied.

TABLE 1.
INPUT FACTORS, RANGE AND UNITS

Input factors	Range	Units
Indium barrier	3 to 15	Å
Channel temperature	445 to 490	°C

CHARACTERIZATION

The goal of these experiments was to develop electron mobility models based on RHEED data recorded during growth of the inverted interface. It has been observed that the interfacial roughness attributable to the bonding type at the InAs–on-AlSb interface impacts electron transport [4]. In addition to its influence on interfacial roughness, bonding type also impacts the material quality of the subsequent thin InAs layer [6], substantiating this study of the InAs RHEED data. Both interfacial roughness and material quality are central issues regarding InAs-AlSb HEMTs.

For each experiment, 5 x 5 mm Hall samples in the clover-leaf van der Pauw pattern were produced and measured at a magnetic field intensity of 3020 Gauss. Hall measurements were taken at temperatures of 300 ºK and 77 ºK. RHEED signals were recorded for each experiment beginning with the Sb soak on the AlGaSb composite layer (Figure 2).

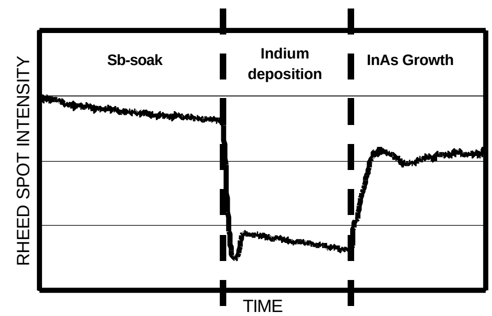


Figure 2. Reflection high-energy electron diffraction (RHEED) signal during InAs/AlSb interface formation.

The RHEED signals are the intensity oscillations observed at the specular spot of the "1X" side of 1 X 3 AlSb Group V-stabilized RHEED pattern. The RHEED data includes intensity oscillations during formation of the interface, as well as growth of the subsequent InAs layer. The process conditions and the results are provided in Table 2.

TABLE 2.
GROWTH PARAMETERS AND 300 °K AND 77 °K MOBILITY RESULTS

INDIUM BARRIER (Å)	CHANNEL TEMP = 460 °C+	77 ºK MOBILITY (cm^2/V/s)	300 ºK MOBILITY (cm^2/V/s)
15	-15	95038	24773
3	30	106792	29356
17.48	7.5	135367	24259
15	30	80257	25716
3	-15	91439	28520
9	39.31	98921	24797
1.3	7.5	101738	31954
9	7.5	137729	28188

NEURAL NETWORK MODELING

Complex relationships exist between film growth conditions and electron transport. The relationships are not well understood, but can be modeled empirically using neural networks, a useful method for mapping relationships between non-linear or noisy data sets. Neural networks have previously been demonstrated to be an effective tool for modeling the effects of MBE process conditions on film qualities [7]. Thus, the process models presented in this paper are developed using this method.

Neural networks are comprised of three basic layers: (1) input, (2) hidden, and (3) output. A diagram of a typical neural network is shown in Figure 3. The network inputs represent the process conditions, and the outputs represent the responses to be modeled. Each layer contains processing elements known as "neurons" interconnected in such a way that information about the relationships between the input and output parameters is stored in the weights between connections. The models presented are developed using the error back-propagation (BP) algorithm [7]. Using this algorithm, input data is first passed through the network using a random set of weights. The output of each neuron is a weighted sum of its inputs, filtered by a sigmoidal "squashing" function. At the final layer, the network outputs and training data are compared, and the mean-squared-error between them is calculated. The error is fed back into the network, where the weights are re-adjusted to minimize the output error. When the network is fully trained, appropriate weights are derived such that the network output represents the relationship between the inputs and outputs of the data set. Networks are typically trained and tested with 75% and 25% of the data set, respectively.

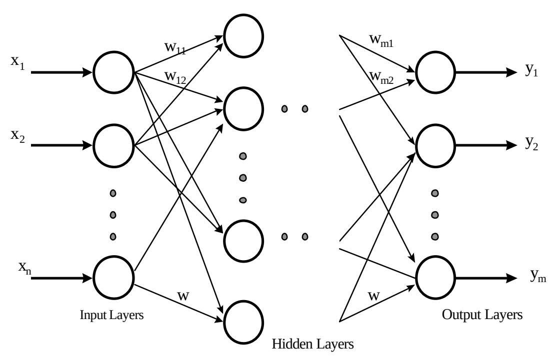


Figure 3. Diagram of neural network

RHEED ANALYSIS

RHEED offers the capability of real-time analysis of the growing surface, thereby making this a useful technique for monitoring the quality of the inverted interface in InAs-AlSb-based HEMTs [8]. This next section presents the mathematical technique used to analyze the RHEED signatures.

PRINCIPLE COMPONENT ANALYSIS

Directly comparing the RHEED signals resulting from different process conditions does not provide information about electron transport or the quality of the interface. Likewise, developing a model based on a time series of RHEED intensity oscillations consisting of hundreds of data points is challenging. Principle component analysis (PCA) is a method that can help overcome some of these difficulties. PCA compresses data into principle components (PCs), which represent the primary components of the variance in the signals [9].

The PCA technique allows the RHEED data to be used to develop process models. Consider a vector **x**, which consists of *p* random variables. Let Σ be the covariance matrix of **x**. Then, for $k = 1,2, \ldots, r$, the *k*th PC is given by

$$z_k = \alpha'_k x$$

where α_k is an eigenvector of Σ corresponding to its *k*th largest eigenvalue λ_k. If α_k is chosen to have unit length (i.e., $\alpha'_k \alpha_k = 1$), then the variance of $z_k = \lambda_k$. Generally, if these eigenvalues are ordered from largest to smallest, then the first few PCs will account for most of the variation in the original vector **x**. In our formulation, we treat each of the sequences of RHEED intensity values as the **x** vectors, and *r* represents the number of intensity values.

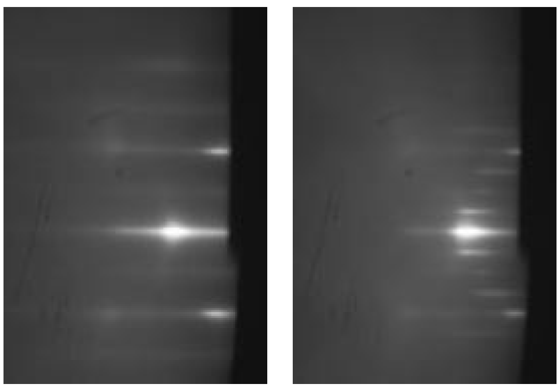
Before PCA was performed on the data, one hundred consecutive intensity values for each RHEED signal were selected beginning with the initiation of the indium deposition. Six PCs were selected, accounting for 99% of the variance in the RHEED signals. The PCA based neural network achieved a 100:6 data reduction ratio while losing less than 1% of the variability in the RHEED signals. These PCs were subsequently used as inputs for a multi-layer neural network, and the electron transport data remain the responses. Neural network process models were developed for 300 °K and 77 °K electron-mobility. The structures and results of the RHEED process models are provided in Table 3.

TABLE 3
RHEED PROCESS MODELS

	300 °K	77 °K
NN Structure	6-5-2-1	6-4-6-1
Training error (%)	0.22	0.46
Testing error (%)	3.78	9.68

RESULTS

Results from the experiments contain excellent room temperature electron-mobility of up to 32,000 $cm^2/V/s$. The process models indicate that the RHEED signals contain information about the quality of the interface as well as the subsequent InAs channel. This makes sense because RHEED patterns are based on reflections from the growth surface, and surface roughness will alter the intensities of the diffraction pattern. This change in the specular spot intensity is observed in the RHEED data. As the indium monolayer(s) are deposited on the Sb-sublayer, the specular spot intensity decreases rapidly. For longer indium soak times, the intensity values reach a point of saturation until the As shutter opens. Once the As shutter opens commencing InAs growth, the intensity increases. As for the RHEED pattern, it changes from a "1X" to a "4X" when the indium soak begins. Afterward, the "4X" changes to a "2X" when InAs growth initiates. The "2X" and "4X" reconstructions (Figures 4a, 4b) can be associated with In- and As-rich growth regimes, respectively.



(a) (b)

Figure 4. RHEED pattern for (a) InAs growth - "2X" and (b) Indium deposition on Sb-sublayer - "4X"

The low temperature results demonstrated a correlation with both indium barrier thickness and temperature, whereas the room temperature results showed a correlation with temperature, only. However, the room temperature model exhibited better accuracy than the low temperature model. This can be attributed to electron-mobility's higher sensitivity to the quality of the interface at lower temperature. [10, 11]. When the indium barrier is thick, the surface becomes saturated with indium, which protects the underlying Sb-sublayer form the ensuing As flux. In addition, too much indium may accumulate on the surface. When the indium barrier is thin, the interface is affected, possibly roughened, as indium desorbs from the interface exposing the Sb-sublayer. With the Sb-sublayer exposed, anion exchange occurs at the interface, where roughness scattering dominates electron-mobility.

SUMMARY

Statistical experimental design was used to explore the effects of the interface formation on device performance parameters. The indium barrier thickness at the inverted, or bottom As/Sb interface was varied from 1 to 5 monolayers and the InAs channel growth temperature was varied from 445 °C to 490 °C. RHEED was used to monitor the interface formation of AlGaSb-InAs-based HEMTs, which were characterized using high and low temperature (300 ^{o}K and 77 ^{o}K) Hall measurements. PCA was performed on the RHEED data, and PCs were chosen to account for 99% of variance that were fed into a multi-layer back-propagation neural network. The PCA-based process models exhibited testing error less than 4% and 10% for 300 ^{o}K and 77 ^{o}K electron-mobility, respectively.

ACKNOWLEDGMENT

The authors would like to acknowledge the support of the Air Force Research Laboratory (F3361598C5428) and State of Georgia Yamacraw Initiative for support of this work.

REFERENCES

[1] W. Barvosa-Carter, M. E. Twigg, M. J. Yang, and L. J. Whitman, "Microscopic characterization of InAs / In0.28GaSb0.72 / InAs / AlSb laser structure interfaces," *Physical Review B*, vol. 63, pp. 1-10, 2001.

[2] B.Z. Nosho, W.H. Weinberg, W. Barvosa-Carter, B.R. Bennett, B.V. Shanabrook, and L.J. Whitman, "Effects of Surface reconstruction on III-V semiconductor interface formation: The role of III/V composition," *Applied Physics Letters*, vol. 74, pp. 1704-1706, 1999.

[3] D. A. Collins, M. Wang, R.W. Grant, and T.C. McGill, "Reflection high energy electron diffraction observation of anion exchange reactions on InAs surfaces," *Journal of Applied Physics*, vol. 75, pp. 259-262, 1994.

[4] G. Tuttle, H. Kroemer and J. English, "Effects of interface layer sequencing on the transport properties of InAs/AlSb quantum wells: Evidence for antisite donors at the InAs/AlSb interface," *Journal of Applied Physics*, vol. 67, pp. 3032-3037, 1990.

[5] G. Box, W. Hunter and J. Hunter, *Statistics for Experimenters*. New York: Wiley, 1978.

[6] B. Z. Nosho, W. H. Weinberg, J.J. Zinck, B.V. Shanabrook, B. R. Bennett, and L. J. Whitman, "Structure of InAs/AlSb/InAs resonant tunneling diode interfaces," *Journal of Vacuum and Science Technology B*, vol. 16, pp. 2381-2386, 1998.

[7] K. Lee, T. Brown, G. Dagnall, R. Bicknell-Tassius, A. Brown, and G. May, "Using Neural Networks to Construct Models of the Molecular Beam Epitaxy Process," *IEEE Transactions on Semiconductor Manufacturing*, vol. 13, pp. 34-45, 2000.

[8] C. R. Bolognesi, I. Sela, J. Ibbetson, B. Brar, H. Kroemer, and J. H. English, "On the interface structure in InAs/AlSb quantum wells grown by molecular beam epitaxy," *Journal of Vacuum Science Technology B*, vol. 11, pp. 868-871, 1993.

[9] I. Jolliffe, *Principal Component Analysis*. New York: Springer-Verlag, 1986.

[10] K. C. Wong, Celeste Yang, Mason Thomas, and Hans-Richard Bland, "Study of the morphology of the InAs-on-AlSb interface," *Journal of Applied Physics*, vol. 82, pp. 4904-4907, 1997.

[11] C.R. Bolognesi, H. Kromer and J.H. English, "Interface roughness scattering in InAs/AlSb quantum wells," *Applied Physics Letters*, vol. 61, pp. 213-215, 1992.

ACRONYMS

HEMT: High electron mobility transistor
RHEED: Reflection high energy electron diffraction
PCA: Principle component analysis
MBE: Molecular beam epitaxy