Neural Network Modeling of Anion Exchange using Reflection High-Energy Electron Diffraction Data

Tomas Sarmiento and Gary S. May
School of Electrical and Computer Engineering
Georgia Institute of Technology
Atlanta, GA. 30332-0250

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Arsenide/antimonide heterostructures have important applications in infrared detectors, lasers, and high-speed electronic devices [1-3]. The performance, and hence, the manufacture of these devices is compromised by the difficulty of controlling the interface properties as a result of the tendency of group V elements to exchange [4]. In this paper, a neural-network based model is developed to enable the control of the As-for-Sb exchange.

The model was constructed by characterizing the As-for-Sb exchange in a set of 20-period "$GaAs_ySb_{1-y}/GaSb$" superlattices (SL) grown by molecular beam epitaxy (MBE) on GaSb (001) substrates. The complete structure is shown in Figure 1. The nominal $GaAs_ySb_{1-y}$ monolayers were formed by the As exposure of an Sb-stabilized GaSb surface and immediate GaSb overgrowth, as illustrated by the shutter sequence depicted in Figure 2. Statistical experimental design was used to efficiently obtain the necessary data for modeling. A D-optimal experiment was implemented to evaluate the effect of different growth parameters on the resulting anion exchange. The growth parameters of interest and their ranges are summarized in Table 1.

Reflection high-energy electron diffraction (RHEED) was used to monitor *in-situ* the surface structure and morphology. In addition, the RHEED pattern along the substrate [110] azimuth was captured and digitally recorded throughout the As exposure.

To quantify the amount of exchange, high-resolution x-ray diffraction $\theta/2\theta$ scans were performed and simulated using dynamical diffraction theory. During the simulations, the thickness of the $GaAs_ySb_{1-y}$ layer was set to two monolayers (MLs), while its composition was adjusted along with the thickness of the GaSb spacers until the simulated data matched the zero-order SL peak position and the SL period.

Due to their inherent ability to learn complex nonlinear relationships, neural networks have been used to model the electron mobility [5] and structural properties [6] of MBE-grown structures. In these cases, features of the RHEED intensity oscillations were extracted and incorporated into the model to improve the prediction accuracy. For real-time applications, it is highly desirable to use the entire RHEED pattern image (instead of RHEED intensity oscillations only) to simplify the data acquisition and feature extraction process.

To incorporate the information provided by the RHEED pattern image into the model, histograms of the images were generated to make the feature extraction simple and fast. The histogram of a typical RHEED pattern image is shown in Figure 3. The histograms of these images exhibit a sharp peak, which is product of the abundant dark pixels of the image. If this peak is removed, the moments of remaining distribution can be used to represent the image. The standard deviation and skew of the distribution represented by the histograms were used, along with the process conditions, as inputs to a neural network. The RHEED images recorded three seconds after the As exposure was initiated were used in the model. A multilayer perceptron neural network with a single layer of hidden neurons was trained using the error back-propagation (BP) algorithm. The training set consists of 13 randomly selected samples, approximately 75% of the data set, while the remaining four samples formed the testing set.

The RMS prediction error was 5.73%. This is illustrated graphically in Figure 4. A model using only the process conditions was also developed. The network was implemented with a similar architecture and was trained and tested with the same training and testing sets. The RMS prediction error of this network was 7.86%, indicating that the incorporation of the RHEED data considerably improves the accuracy of the model. The structure and prediction error of each neural networks are summarized in Table 2.

Following the methodology presented, similar models can be developed to predict the amount of As-for-Sb exchange in arsenide/antimonide structures from the RHEED patterns. This will potentially allow run-to-run and/or real-time control of the exchange enhancing the manufacture of devices that contain arsenide/antimonide heterointerfaces.

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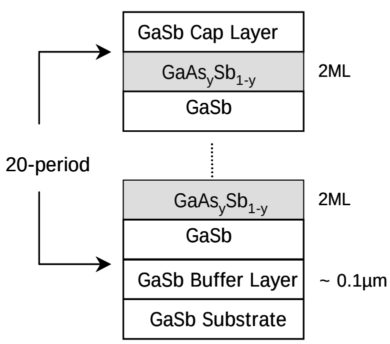

Figure 1. Nominal structure of the 20-period "$GaAs_ySb_{1-y}$/GaSb" superlattice. A ~ 1µm thick GaSb buffer layer and a GaSb cap layer complete the structure.

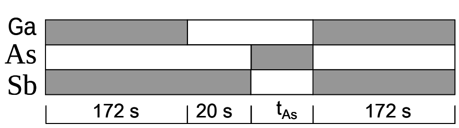

Figure 2. Shutter sequence used for the formation of the nominal $GaAs_ySb_{1-y}$ monolayers. The As exposure time t_{As} was set between 10 and 30 s.

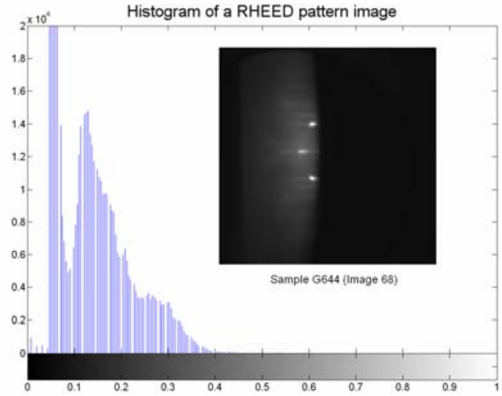

Figure 3. Histogram of a typical RHEED pattern image

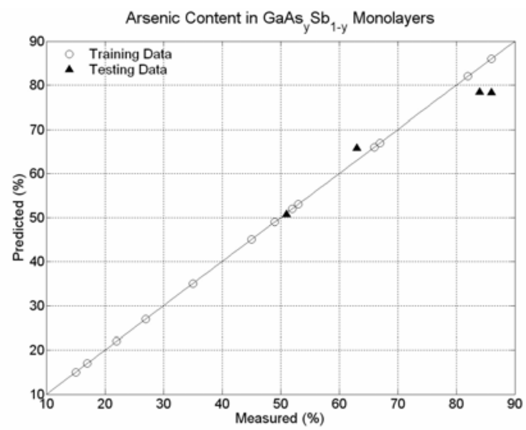

Figure 4. Neural network modeling results. The solid triangles correspond to the testing data and the open circles correspond to the training data.

Table 1. Growth parameters considered in the experiment.

Parameter	Range
As species	As_2, As_4
Exposure time (t_{As})	10-30 s
Substrate temperature (T_S)	400-440 °C
As flux pressure (P_{Asx})	2 µTorr, 4 µTorr
Sb flux pressure (P_{Sb2})	2 µTorr, 4 µTorr

Table 2. Neural network structures and prediction errors. Model 1 uses both the process condition and the RHEED pattern data while model 2 uses only the process conditions. The notation "i-j-k" refers to the number of input, hidden layer, and output neurons, respectively.

	Model 1	Model 2
NN Structure	7-4-1	5-3-1
NN RMS Testing Error (%)	5.73	7.86