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Computational intelligence applied to the growth of quantum dots

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ABSTRACT

We apply two computational intelligence techniques, namely, artificial neural network and genetic algorithm to the growth of self-assembled quantum dots. The method relies on an existing database of growth parameters with a resulting quantum dot characteristic to be able to later obtain the growth parameters needed to reach a specific value for such a quantum dot characteristic. The computational techniques were used to associate the growth input parameters with the mean height of the deposited quantum dots. Trends of the quantum dot mean height behavior as a function of growth parameters were correctly predicted and the growth parameters required to minimize the quantum dot mean height were provided.

1. Introduction

The last decade has witnessed the development of semiconductor quantum dot (QD) structures for application in a variety of optoelectronic devices [1,2]. QDs are structures on the nanometer scale, which confine the electrons in all three dimensions, leading to the full quantization of the electronic energy levels. The performance of many optoelectronic devices can greatly benefit from the fact that the electronic energy levels are fully quantized [2]. In particular, QD structures have shown a great potential to outperform the quantum well structures in the development of infrared photodetectors based on intraband optical transitions, due to the three-dimensional confinement [2,3]. Efficient coupling of the normal incident light and higher operation temperatures are some of the promised advantages of the QD structures. Whether the predictions in terms of improved performance of the infrared photodetectors will prove to be realistic or not, strongly depends on the growth of QD structures with high dot density, small size and small size dispersion. One of the difficulties in the process of QD growth is to set up the growth parameters to reach a specific characteristic, namely: a certain QD mean height or density or both. Computational intelligence techniques such as artificial neural network (ANN) and genetic algorithm (GA) may be helpful in finding the optimal growth conditions to achieve a desired QD structure. The use of ANN has already been considered crucial to solve the future challenges of epitaxial growth [4]; however, to the authors' knowledge no results have yet been published.

In this work, we have used computational intelligence techniques to predict trends in the InAs QDs' mean height behavior as a function of different growth parameters. In addition, we have obtained the growth conditions such that the QD mean height should be minimized.

2. Experimental details

The investigated samples contain one layer of free standing self-assembled InAs QDs deposited by metalorganic vapor phase epitaxy (MOVPE) at 100 mbar on top of InP, InGaAs or InGaAlAs, where the alloys are all lattice matched to the InP substrate. Equivalent structures have been used in the development of QD infrared photodetectors, and are described in great detail elsewhere [5]. The QD height and density of the grown samples were determined by atomic force microscopy (AFM). X-ray diffraction and conventional photoluminescence were used to determine the alloy composition.

3. Computational intelligence

Computational intelligence is a branch of computer science that develops algorithms and techniques to imitate some cognitive abilities, like recognition, learning and evolution. Some of those techniques are ANN and GA. ANNs are widely used in problems of series prediction, recognition of standards and

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function approximation [6]. It is a non-linear mathematical model used to find complex relationships between input and output. The main advantage of ANN over other interpolation methods is its capability of modeling systems with a very strong non-linear behavior. Even though it is not possible to extract deep physical insights on the growth mechanisms from the ANN, one can obtain trends that can help in constructing new physical models or in understanding the growth procedures, as we demonstrate ahead in this article.

GA is an algorithm of search and optimization with wide and successful applications in several areas [7]. It is an iterative algorithm that belongs to a group of techniques inspired in Darwin's natural selection principle. These algorithms use a process based on genetic reproduction to achieve an optimal or sub-optimal solution of a problem. The procedure is as follows: each possible solution in a problem is modeled and codified in a string of bits or symbols. Such structure is known as "chromosome". Thus, each of these chromosomes represents an individual or a solution, which is evaluated according to predetermined criteria and receives a score that informs how good a particular individual (solution) is for the problem. In the sequence, individuals are chosen based on their score, in a way that individuals with higher scores have a larger probability of being chosen. The selected individuals are combined and new ones are generated. The new individuals are expected to be better or, at least, as good as their generators. The new individuals replace the ones with low scores, and the process restarts. The procedure is repeated until a stop condition is reached, which is often the number of cycles.

The idea in this reported work is to use an existing database of growth parameters with the resulting QD mean height to be able to supply the set of growth parameters needed to reach a desired QD mean height. Note that any other sample characteristic could have been chosen. In order to do so we first use an ANN to infer the behavior of the nucleated QDs. Subsequently, we apply the GA technique to obtain the parameters' configuration (set of growth parameters) which will lead to a desired mean height of the QD. We have used a total of 67 sets of growth parameters and chose to minimize the QD mean height, as much as possible.

The six different growth parameters of each set used as input to create the ANN are: the indium flux in the reactor, the growth temperature, the deposition time, the width of the layer on top of which the dots are nucleated, the aluminum and indium contents of this layer material. We have used three different materials for this substrate layer, namely, InP, InGaAs and InAlGaAs. The network output is the mean QD height. Obviously, the QD height depends on other parameters such as pressure and annealing time, for instance. However in our database these parameters were kept constant, consequently using them as input for the ANN is unnecessary in this case. When necessary, any other parameter can be introduced in the creation of the neural network.

The ANN modeling algorithm is an iterative process where on each step one set of growth parameters, contained in our database, is introduced in the ANN. The ANN computes the difference between its obtained output and the corresponding experimental QD height. So the ANN configuration is adjusted following a minimization error method, with the purpose of reducing this difference. This process is repeated until a predefined error is reached. At this point, the ANN is ready to be used as a function that is able to mimic the QD growth process. Some data points are reserved to be used to validate the model.

Once the neural network was created, validated and tested, we have combined it with the GA, enabling us to obtain the growth parameters which are, in principle, most suitable for minimizing the QD mean height. This is accomplished by using an ANN to infer the behavior of the QDs, and after that, the GA technique to obtain the parameters' configuration which leads to the minimum QD mean height possible, given the growth parameters' ranges used as input to the ANN.

4. Results and discussion

In Fig. 1, the error histogram for the created ANN is shown. Around 90% of the evaluated cases predict an error below 20%, a result that reveals an excellent accuracy of the network.

Fig. 2 depicts in red the QD mean height obtained by the neural network for the 67 different sets of growth parameters. In the same figure we observe in black the experimental values obtained by AFM images. The results obtained by the ANN follow quite closely the experimental data. In fact, in the testing stage of the establishment of the ANN (highlighted in grey in Fig. 2), a mean average percentage error of only 8.3% is achieved, which is an exceptional result given the relative small number of sets of growth parameters used as input for the creation of the network.

With the generated ANN, we have used the GA to find the set of growth parameters that can minimize the QD height for the

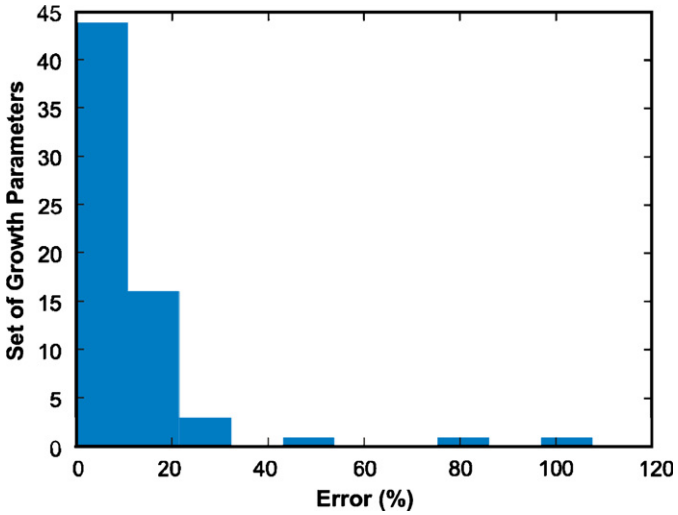

Fig. 1. Histogram of the neural network with the percentage error for all sets of growth parameters used as input to the network.

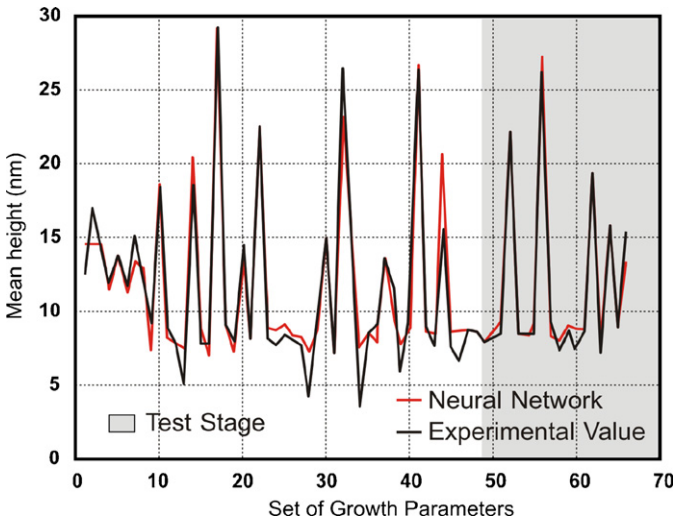

Fig. 2. Comparison of the ANN prediction for the QD mean height and the obtained experimental data obtained by AFM.

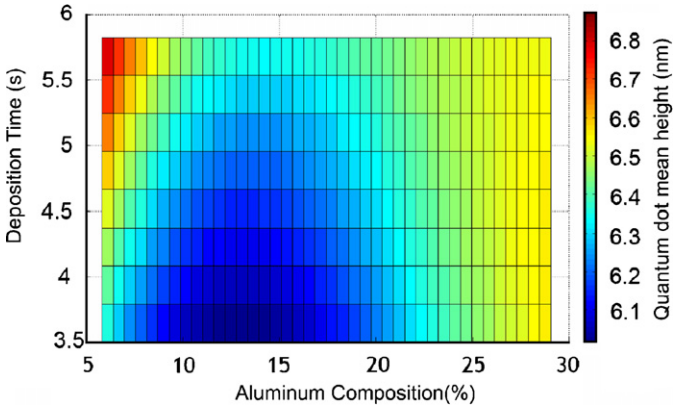

Fig. 3. Effect of aluminum composition and deposition time on the QD mean height.

investigated materials. In our calculations, 500 cycles of the GA were applied, even though after around 200 cycles the GA already converged to a minimum QD mean height, demonstrating the efficiency of the procedure. The growth parameter configuration obtained to achieve the smallest possible QD mean height with the MOVPE reactor used is: In flux equal to 60.0 sccm, InGaAlAs thickness of 1.5 nm, substrate temperature equal to 519.8 °C, deposition time of 2.4 s and In and Al content in the InGaAlAs alloy material equal to 53.44% and 21.79%, respectively. This set of growth parameters should lead to a QD mean height of 4.5 nm. A sample using these growth conditions should soon be grown.

Another interesting and useful application of the ANN to the growth of the investigated QDs is the possibility to visualize how each growth parameter influences the QD mean height. This can be accomplished, for instance, by fixing four input parameters of the ANN and analyzing how two others affect the output. In Fig. 3 we show the effect of the Al content in the InGaAlAs alloy layer (lattice matched to the InP substrate) on top of which the QDs were deposited and of the deposition time on the QD mean height. We have assumed an In flux of 60 sccm, an In content in the quaternary layer of 52.3% and thickness of 500 nm, and a growth temperature of 500 °C.

We can see in Fig. 3 a clear tendency of reduction in the QD mean height as the Al content in the alloy increases up to about 13%. For larger Al content, the QD mean height increases continuously. This behavior has already been experimentally observed, and a minimum QD size was reached for 16% Al content in the InGaAlAs alloy lattice matched to InP [8]. These previously published results are in excellent agreement with our data, especially if we consider the small number of input parameters used in the creation of our ANN. In the same figure, one can observe that the QD mean height increases with deposition time, as expected, since the QDs have more time to grow. Our results unambiguously demonstrate that the ANN not only provides appropriate information on the QDs' mean height for a specific growth configuration, but it also predicts the trends of the mean QD height as a function of different growth parameters.

5. Conclusion

We have demonstrated the enormous potential of computational intelligence techniques in guiding the growth of QDs. It is encouraging that even with a rather small database we have obtained results with very good accuracy, suggesting that the ANN can be a reliable approximation of the function that governs the growth of QDs, provided a wide range of sets of input data is available.

Even though the results reported here are specific for a particular QD characteristic, it is clear that the computational techniques reported here can be used to predict any desired sample parameter or trend in different samples' characteristics. We have also studied the QD density with great success. Another interesting characteristic to be studied would be QD size dispersion, which is already underway.

Computational techniques such as the ones employed in this investigation decrease the number of experiments needed in laboratory, as they serve as a guide in searching for growth parameters, reducing research costs. The obtained preliminary results are quite promising, in particular for industrial applications, and show how the development of the nanotechnology can greatly benefit from the judicious use of computational techniques.

Acknowledgments

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