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Computational modeling of isothermal decay curves of trapping centers in TlGaSeS layered single crystals

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ABSTRACT

This paper presents a new approach based on multilayered perceptrons (MLPs) to compute the isothermal decay curves of trapping centers in undoped TlGaSeS layered crystals. The MLP has been trained by a Genetic Algorithm (GA). The results obtained using the MLP model were tested with an untrained experimental data. The comparison has shown that the proposed model can predict more accurately and easily the isothermal decay curves.

1. Introduction

The crystal TlGaSeS of layered semiconductors is formed from $TlGaS_2$ and $TlGaSe_2$ crystals by replacing half of the sulfur (selenium) atoms with selenium (sulfur) atoms [1,2]. These crystals are useful for optoelectronic applications as they have high photosensitivity in the visible range of the spectra and high birefringence in conjunction with a wide transparency range of 0.5–14.0 μm [3–10].

One of the determining factors in the eventual device performance of semiconductors is the presence of impurity and/or defect centers in the crystal. Thus, it is very useful to get detailed information on energetic and kinetic parameters of trapping centers (hole traps in the present paper) in semiconductor in order to obtain high quality devices. Among the several experimental methods for determining the properties of trap centers in semiconductors, thermally stimulated current (TSC) measurements are relatively easy to perform and provide detailed information on trap states [11–19].

The isothermal method is one of several methods to evaluate the trapping parameters from the experimental TSC spectra. In this method, the sample is heated at a constant rate from T_0 to T_p and then held at T_p until complete detrapping. For this process, the thermally stimulated current can be described by [11]

$$I = I_0 \exp(-\gamma t) \quad (1)$$

where I_0 is the initial current at time $t = 0$, $\gamma = \nu \exp(E_t/kT_p)$, ν is the attempt-to-escape frequency and E_t is the activation energy. The TSC decay measurements on the TlGaSeS crystal were repeated at temperatures T_p = 24, 29, 34, 39, 46 and 51 K. Thus, a series of slopes (γ values) of the plots ln(I) versus time t are obtained for each temperature T_p. The ln values of the slopes versus $1/T_p$ give a straight line from which E_t was obtained. The linear intersection of the ln(γ) versus $1/T_p$ graph gives the attempt-to-escape frequency.

The generalization ability, real-time operation, and ease of application have made artificial neural network (ANN) quite popular in the last years [20]. ANNs have been applied in many areas because of these features [21–26]. The ANN software available today provides many neural network architectures and learning algorithms, to be applied for the specific problems.

The purpose of the present work is to model the isothermal decay curves of trapping centers in undoped TlGaSeS layered crystals using GA, ANNs and experimental data. The proposed model

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is not time consuming and more accurately and easily predicted the isothermal decay curves in as-grown TlGaSeS layered single crystals.

2. Experimental details

TlGaSeS polycrystals were synthesized from high-purity elements prepared in stoichiometric proportions. Single crystals of TlGaSeS were grown by the Bridgman method. The resulting ingot appears red in color and the freshly cleaved surfaces were mirror-like. For TSC measurements a sample with dimensions of 9 mm × 10 mm × 0.5 mm were used. Electrical contacts were made on the sample surface with silver paste according to "sandwich" geometry. In this configuration, the electrodes are placed on the front and back sides of the crystal. Thin copper wires were attached to the electrodes for circuit connection. The electrical conductivity of the studied sample was p-type. The sample was mounted on the cold finger of the cryostat.

The TSC measurements were performed in the temperature range from 10 to 100 K and using a closed-cycle helium cryostat. Constant heating rate of 0.8 K/s was achieved by a Lake-Shore 331 temperature controller. A Keithley 228A voltage/current source and a Keithley 6485 picoammeter were used for the TSC measurements. The nominal instrumental sensitivities of temperature and current measurement devices were about 10 mK and 2 pA, respectively.

3. Multilayered perceptron neural networks

There are many types of neural networks for various applications available in the literature. Multilayered perceptrons (MLPs) are feed-forward networks and universal approximators. MLPs are the simplest and therefore most commonly used neural network architectures [20]. In this paper, they have been adapted for the computation of the isothermal decay curves of trapping centers in undoped TlGaSeS layered crystals.

The MLP used in this work is trained with the GA. An MLP consists of three layers: an input layer, an output layer, and an intermediate or hidden layer. Processing elements (PE) or neurons in the input layer only act as buffers for distributing the input signals x_i (i show the ith input PE) to PEs in the hidden layer. Each PE j (j show the jth PE in the hidden layer and output layers) in the hidden layer sums up its input signals x_i after weighting with the values of the respective connections w_{ji} from the input layer and computes its output y_j as a function f of the sum,

$$y_j = f\left(\sum w_{ji} x_i\right) \quad (2)$$

f can be a simple threshold function, a sigmoid or hyperbolic tangent function. The output of PEs in the output layer is computed similarly. Training a network consists of adjusting its weights using a training algorithm. The training algorithms adopted in this study optimize the weights by attempting to minimize the sum of squared differences between the desired and the actual values of the output neurons [20], namely:

$$E = \frac{1}{2}\sum_j (y_{dj} - y_j)^2 \quad (3)$$

where y_{dj} is the desired value of output neuron j and y_j is the actual output of that neuron. Each weight w_{ji} is adjusted by adding an increment Δw_{ji} to it. Δw_{ji} is selected to reduce E as rapidly as possible. The adjustment is carried out over several training iterations until a satisfactorily small value of E is obtained or a given number of iterations are reached. The computed Δw_{ji} depends on the training algorithm adopted. There are a number of training algorithms used to train a MLP and a frequently used one is called the back-propagation (BP) training algorithm [20]. The BP algorithm, which is based on searching an error surface using gradient descent for points with minimum error, is relatively easy to implement. However, the BP algorithm has some problems for many applications [27]. The algorithm is not guaranteed to find the global minimum of the error function since gradient descent may get stuck in local minima, where it may remain indefinitely. In addition to this, long training sessions are often required in order to find an acceptable weight solution because of the well-known difficulties inherent in gradient descent optimization [27].

In this work target current (I) for the MLP has been determined by GA. The computation process is carried out with a set of TSC measurements.

4. Determination of target current with genetic algorithm

The GA method is based on a computer simulation of biological evolution and initially works with a randomly generated population with several variables to be estimated [28]. The population size is usually related to the problem under consideration and can be determined by a number of variables. Each member or individual of the population is usually called a chromosome or a string consisting of genes or bits, and encoded into one variable (I) for this work. A new population is built up by selecting individuals among members of the initial population according to their fitnesses through fundamental genetic process of selection criterion based on the roulette wheel. The fitness function (ff) is calculated by

$$ff = \frac{1}{\sum_{k=1}^{n} (I_{t\_d,k} - I_{t\_c,k})^2} \quad (4)$$

where n is the population size, I_{t_d} and I_{t_c} are the desired and computed current, respectively.

Fitness value for each string was calculated using the fitness function, hence new members were chosen for reproduction according to their fitness based on the specified selection criterion. Thus, the fittest had a greater chance to be selected for next population. Once the reproduction was completed crossover operation was implemented by simply exchanging bits between two randomly selected members in the population. The final genetic process was mutation that randomly changes a particular bit in a particular string, that is, a zero bit may change to a one or vice versa.

5. Results and discussion

The proposed technique involves training an MLP to compute the current for isothermal decay curves when the values of slope (s), maximum current (I_{max}), time (t), and temperature hold (T_h) are given. The ranges of training data set were $0.00479 \le s \le 0.07433$ at 5 points, 6.11 μA ≤ I_{max} ≤ 28.44 μA at 5 points, 7.93 s ≤ t ≤ 249.47 s at 489 points, 24 K ≤ T_h ≤ 51 K at 5 points. The current configuration to be modeled by the neural network is shown in Fig. 1. Training an MLP using the GA to compute I involves presenting them with different sets (s, I_{max}, t and T_h) sequentially and/or randomly and corresponding calculated values I. Differences between the target output (I) and the actual outputs ($I_{\_ANN}$) of the MLP are calculated through the network to adapt its weights using Eqs. (2)–(4). The adaptation is carried out after the presentation of each set (s, I_{max}, t and T_h) until the calculation accuracy of the network is found satisfactory according to some criterion (for example, when the

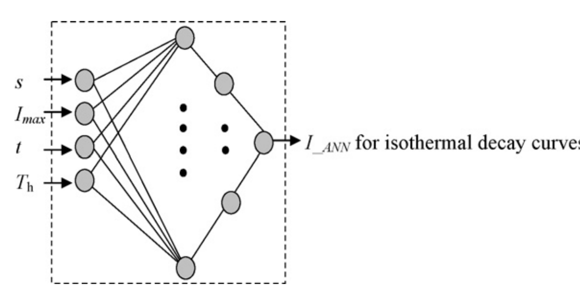

Fig. 1. Neural calculation for isothermal decay curves of trapping centers from the thermally stimulated current.

errors between I and I_{-ANN} for all the training set fall below a given threshold) or the maximum allowable number of epochs (the time periods that encompasses all the iterations performed after all the patterns are presented to the network) is reached.

Furthermore, in order to understand the MLPs prediction accuracy and generalization capacity the networks were also trained with the training set, cross-validation set and checked with test data. The network memorizes the training set and does not generalize well when the network is trained too much [27]. The training holds the key to an accurate solution, so the criterion to stop training must be very well described. Cross-validation is a highly recommended criterion for stopping the training of a network. When the error in the cross-validation increases the training should be stopped. A practical way to find a point of better generalization is to use a small percentage (around 10%) of the training set for cross-validation. For obtaining a better generalization of the networks presented in this work 293 of training data, which were selected randomly, were used as cross-validation set.

Total 2934 data sets were used in training and test phases. Fig. 2 shows the current values versus the network outputs for all training data set. The diagonal line in this graph shows perfect match between measurement and network output. 398 data sets were used to test the network. For the validation, untrained experimental data are also used to test the neural model as well. The number of hidden layers and neurons in each layer were determined through trial and error to be optimal including with different transfer functions as hyperbolic tangent, sigmoid and hybrid. The MLP was also trained by the BP learning algorithm to compare with the GA. Table 1 presents training times (for Intel Centrino™ 1.6 GHz with 512 MB of RAM) for training algorithms and errors of different topologies of MLPs trained by the BP and GA for 1000 epochs. It can be clearly seen from Table 1 that the GA algorithm provided a more performance as being the more accurate algorithm than the BP algorithm. After trials, a better result was obtained from the network a four-layered network as seen in Table 1. In this network the hyperbolic tangent function is used in the hidden layers, and sigmoid function is used in the output layer. The number of epochs was 1000 for training, and the most suitable network configuration found was $4 \times 48 \times 24 \times 1$. It means that the number of neurons were 48 and 24 for the first hidden layer and second hidden layer, respectively.

In the proposed model 6 isothermal decay curves of trapping centers in undoped TlGaSeS layered single crystals were used. The estimates of I were found to be in a range from 26.34 to 0.001 μA by use of measured current results in the TlGaSeS layered single crystals at hold temperatures varying from 24 to 51 K. The correlation coefficient for the trained data was found to be 0.9997.

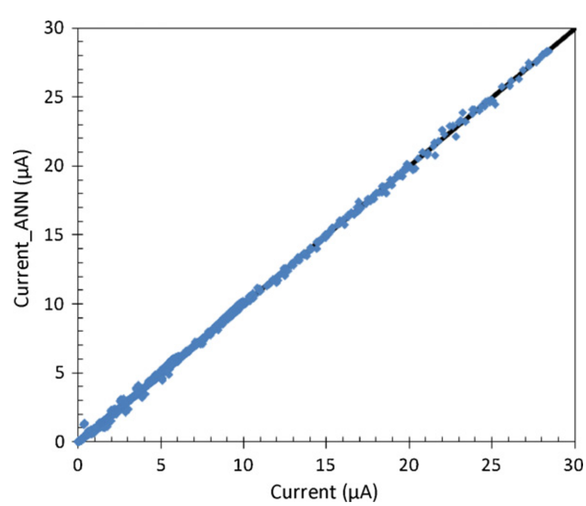

Fig. 2. Plot of the measurement current values versus the network outputs.

Table 1
Different topologies of MLPs trained by BP and GA.

Training algorithm	The number of neurons in		Training time (min:s)	Error
	First hidden layer	Second hidden layer		
BP	6	–	00:45	0.00925
	12	–	01:20	0.00854
	24	–	02:11	0.00750
	48	–	04:05	0.00543
	96	–	06:10	0.00550
	6	4	06:50	0.01517
	12	6	08:40	0.01315
	12	12	10:25	0.00825
	24	12	13:42	0.00310
	48	24	14:15	0.00098
	96	48	15:24	0.00195
	96	24	19:30	0.00220
GA	6	–	01:50	0.00020
	12	–	02:43	0.00015
	24	–	05:45	0.00010
	48	–	08:12	0.00005
	96	–	10:05	0.00008
	6	4	07:10	0.00109
	12	6	14:50	0.00050
	12	12	15:35	0.00001
	24	12	17:05	4.50×10^{-5}
	48	24	15:25	6.59×10^{-6}
	96	48	30:10	1.23×10^{-5}
	96	24	25:23	0.00021

All tested isothermal decay curves of TlGaSeS crystal in the range of training data have high correlation coefficients. Fig. 3 shows the variation of curves obtained from the neural network model and experimental data. The values of current achieved from the proposed model are in good agreement with the experimental values of the TSC. The model was assessed by hold temperature at 34 K which is outside the training data. The variation of the isothermal decay curves for hold temperature at 34 K with time given in Fig. 4 also shows good correlation between measured and predicted results. The correlation coefficient for the untrained data was found to be 0.9889.

The proposed method has some inherent limitations which make it not a general solution. The trained neural network is based on a specific set of TlGaSeS layered single crystals. The trained network can be only valid for the same single crystals. For different single crystals, a series of experiments would have to be performed again to obtain input data for the proposed ANN training. If the ANN

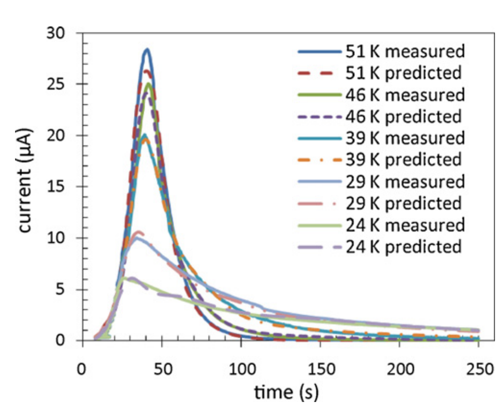

Fig. 3. Variation of predicted and measured isothermal decay curves with time for TlGaSeS crystal at different hold temperatures.

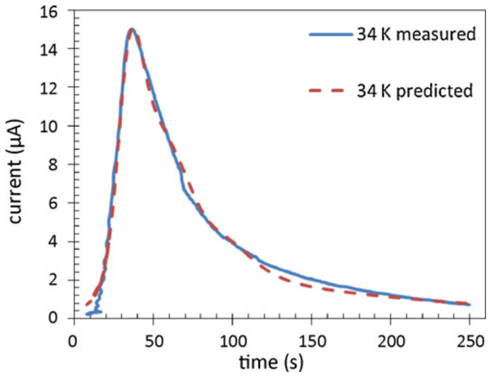

Fig. 4. Comparisons of the predicted and measured isothermal decay curves at 34 K hold temperature.

input data could include the TSC information of new single crystals, many more experimental data would have to be done to meet the accuracy requirements for a more general solution. However, since the neural model presented in this work has accuracy and requires no tremendous computational efforts and less background information about the TSC, it can be very useful for the layered single crystals. This model capable of more accurately predicting isothermal decay curves of trapping centers in as-grown TlGaSeS layered single crystal is also very useful to researcher working in this field.

6. Conclusions

The isothermal decay curves can be predicted by the MLPs using TSC measurements. The predicted currents can be used for computation of the isothermal decay curves based on the TSC method and this helps to obtain a better understanding of the isothermal decay curves of trapping centers with hold temperatures. Finally, the results shows that the proposed model can be useful tool for researcher to assess the isothermal decay curves of trapping centers in TlGaSeS layered single crystal performance.

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