MODELING AND PREDICTION OF THE ELECTRICAL CONDUCTIVITY OF SEMICONDUCTOR NANOTUBES USING ARTIFICIAL NEURAL NETWORKS

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In this study, the dependence of the electrical conductivity of semiconductor nanotubes (SNTs) on key parameters-temperature, doping level, and diameter-was modeled and predicted using an artificial neural network (ANN) approach. A semi-empirical model was used to generate 2,000 synthetic data samples, and based on these, an ANN was implemented in the TensorFlow/Keras framework. The results indicate that as temperature increases, enhanced phonon scattering leads to a decrease in conductivity, whereas increases in doping concentration and nanotube diameter result in higher conductivity due to an increased number of charge carriers and reduced surface scattering.

Keywords: semiconductor, nanotube, neural network, machine learning
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1. INTRODUCTION

Semiconductor nanostructures occupy a very important place in modern materials science and nanoelectronics. These nanomaterials differ from conventional semiconductors by their physical and chemical properties at the nanoscale, and their unique characteristics form the foundation for future technological innovations. In particular, nanowires, nanotubes, quantum dots, and similar nanostructures are widely used to enhance the performance of electronic and photonic devices [1].

The most commonly used for electrical conductivity,

$$\sigma = q(n\mu_n + p\mu_p) \quad (1)$$

is one of the fundamental relations of classical semiconductor physics, where q is the elementary charge; n and p are the electron and hole concentrations, respectively; and μ_n and μ_p are their mobilities. Electrical conductivity is one of the key parameters determining the functionality of a SNTs [2]. This parameter is closely linked to the mobilities and concentrations of electrons and holes, as well as to the interactions among these charge carriers.

Reducing the dimensions of a nanowire confines the free motion of electrons, leading to the quantization of energy levels and the emergence of tunneling effects. Consequently, in SNTs the parameters in equation (1) can no longer be treated as simple constants. Electrical conductivity in SNTs therefore exhibits nonlinear and complex dependencies that differ markedly from those predicted by classical models. As a result, traditional classical theories struggle to fully and accurately describe the conductivity of these systems.

Moreover, electrical conductivity can be influenced by a large number of variables (temperature, pressure, morphology, atomic arrangement, etc.), which may also interact with one another. In such high-dimensional systems, obtaining reliable results with classical statistical models becomes difficult, making the application of machine learning methods necessary. ANNs are capable of modeling complex relationships, learning from the random variability in data, and generalizing effectively [3–5]. These capabilities make ANNs an ideal tool for studying the electrical conductivity of semiconductor nanostructures [6].

In this study, we aim to model and predict the electrical conductivity of SNTs using ANNs, taking into account the variability of key parameters-temperature, nanowire diameter, and doping level-within specified intervals. This approach seeks to deliver accurate, realistic results by explicitly incorporating uncertainties and parameter fluctuations.

2. THEORETICAL FOUNDATIONS AND METHODOLOGY

In real experimental conditions, parameters such as temperature, doping level, and nanostructure dimensions are not perfectly constant but exhibit some variability. Moreover, owing to measurement uncertainty and material heterogeneity, electrical conductivity is often specified as an interval. Representing these parameters as intervals ensures that the model delivers accurate and reliable predictions across all plausible scenarios and enhances the ANN's generalization capability [7-9].

The first step toward accurately predicting electrical conductivity with an ANN is the collection and preprocessing of a synthetic dataset. This dataset may be derived from experimental results or from computational (simulation or theoretical) studies. In the present work, the synthetic parameter ranges are defined as follows:

- Temperature (T): 280–350 K, covering room temperature (298 K) up to elevated temperatures relevant for low-heat-flux and phonon-scattering regimes.
- Diameter (d): 48–52 nm, representative of typical multi-walled nanotubes or large single-walled nanowires, chosen narrow enough to reveal nonlinear effects.

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➢ Doping concentration (N): (0.95–1.05) × 10^{18} cm^{-3}, corresponding to a "light–moderate" active doping level that strongly influences conductivity.

To ensure that the ANN's conductivity predictions reflect physically meaningful trends rather than random noise, we employ the following semi-empirical model as the data-generation basis:

$$\sigma(T,d,N) = qN\mu_0\left(\frac{T_0}{T}\right)^{\alpha}\left(1+\beta log\left(\frac{d}{d_0}\right)\right)+\varepsilon \quad (2)$$

where μ_0- is the referency mobility, α-temperature exponent, β-diametr-correction coefficient, T_0 and d_0 normalization constants, and ε-denotes a random variation term.

An ANN architecture was then constructed to estimate σ. Modeling was performed in Python using TensorFlow and the Keras API. The network comprises three input nodes (T, N, d), two hidden layers with ReLU activation functions, and a single output node (σ). This configuration provides sufficient depth and flexibility to capture the nonlinear dependencies and high-dimensional interactions typical of materials science data. ReLU accelerates training convergence and improves stability.

A synthetic dataset of 2,000 samples was generated according to equation (2), ensuring both physical realism and statistical variability. All inputs were normalized prior to training to promote faster and more stable convergence. Early stopping and validation-loss monitoring were employed to prevent overfitting.

3. NUMERICAL RESULTS AND DISCUSSION

On the held-out test set, the ANN achieved high-precision conductivity predictions. The coefficient of determination, R^2, exceeds 0.95, demonstrating strong generalization and a robust learned relationship between inputs and output. Error metrics such as Mean Absolute Error (MAE) and Mean Squared Error (MSE) remained low, confirming that the predicted conductivities closely match the semi-empirical baseline values. All results were evaluated within 95% confidence intervals, and the observed statistical variations during training fell within acceptable bounds. These performance indicators confirm that the model operates stably and produces physically consistent results.

Figure 1 presents the three principal plots derived from the model's outputs, illustrating the effects of temperature, doping concentration, and nanotube diameter on electrical conductivity.

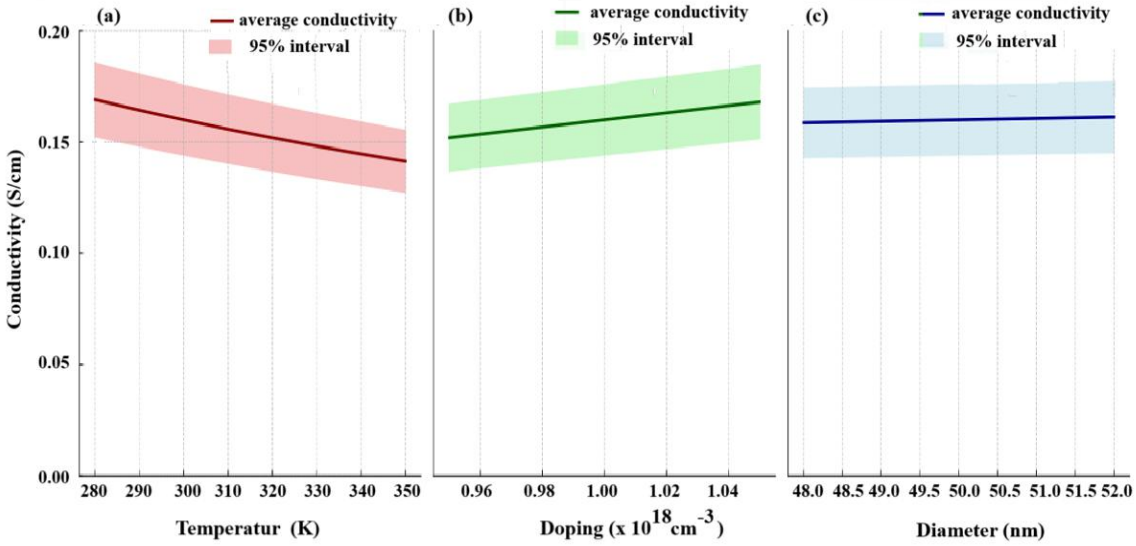

Fig. 1. Effects of parameters on the electrical conductivity of SNT: (a) temperature dependence, (b) doping dependence, (c) diameter dependence. Parameters: $\mu_0 = 0.01$ m²/(V·s), $\alpha = 0.8$, $\beta = 0.2$, $T_0 = 300$ K, $d_0 = 50$ nm, $\varepsilon = 5$ %.

Within the model framework, conductivity decreases as temperature increases. This behavior is characteristic of SNTs and nanowires and is primarily attributed to enhanced phonon scattering: at higher temperatures, the increased phonon population leads to more frequent carrier scattering, which reduces carrier mobility and thus lowers the overall electrical conductivity [13]. However, this is not universal for all materials and structures. In some lightly doped nanosemiconductors with narrow bandgaps, thermal activation at elevated temperatures can increase the carrier concentration; even if mobility decreases, the net effect may be an increase in conductivity. Such behavior is observed particularly in certain intrinsic semiconductors and nanostructures.

As the doping concentration increases, a corresponding rise in electrical conductivity is observed. This is explained by the fact that doping

increases the number of free charge carriers (electrons or holes) in the material. A higher carrier density enhances the overall charge transport capability, leading to higher conductivity values—as seen, for example, in carbon nanotubes. In the model, since carrier mobility is held constant, the relationship between doping level and conductivity is represented by a monotonically increasing line.

When the nanotube diameter increases, a slight but consistent increase in electrical conductivity is observed. This effect is mainly due to reduced surface scattering and weakened quantum confinement. In wider-diameter structures, electrons experience fewer boundary collisions, resulting in less scattering and therefore higher conductivity. Although this increase is not dramatic, it is a clear trend within the examined parameter range.

4. CONCLUSION

In this study, we have effectively modeled and accurately predicted the complex, nonlinear relationships between electrical conductivity and its governing parameters in SNTs. Explaining the simultaneous, nonlinear influence of three variables—temperature, doping, and diameter—on conductivity is challenging with classical models alone. Therefore, we applied an ANN approach. The ANN is capable of learning complex interactions among these variables and predicting conductivity with high accuracy. By capturing the combined effects of temperature, doping, and diameter, the model accounts for intricate behaviors that simple analytical models cannot cover. We found that conductivity generally decreases with increasing temperature due to stronger phonon scattering, although thermal activation can lead to increases in some structures. Conductivity also increases with both doping level and diameter.

The application of ANNs proved valuable for exploring scenarios beyond the reach of classical models, and this approach is recommended as an effective tool for deeper understanding and prediction of the functional properties of semiconductor nanowires [14,15].

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