



An embedded simulation approach for modeling the thermal conductivity of 2D nanoscale material



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ABSTRACT

The thermal property of single layer graphene sheet is investigated in this work by using an embedded approach of molecular dynamics (MD) and soft computing method. The effect of temperature and Stone–Thrower–Wales (STW) defects on the thermal conductivity of graphene sheet is first analyzed using MD simulation. The data obtained using the MD simulation is then fed into the paradigm of soft computing approach, multi-gene genetic programming (MGGP), which was specifically designed to model the response of thermal conductivity of graphene sheet with changes in system temperature and STW defect concentration. We find that our proposed MGGP model is able to model the thermal conductivity of graphene sheet very well which can be used to complement the analytical solution developed by MD simulation. Additionally, we also conducted sensitivity and parametric analysis to find out specific influence and variation of each of the input system parameters on the thermal conductivity of graphene sheet. It was found that the STW defects has the most dominating influence on the thermal conductivity of graphene sheet.

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1. Introduction

Graphene is a 2-dimensional nanomaterial which has attracted significant research interest in material science due to its attractive physical and mechanical properties [1,2]. Ever since it was discovered [3], the exceptional qualities of graphene has been widely studied and investigated to explore its diverse possible applications in real world. These include applications in electric circuits such as graphene-based integrated circuits (ICs), field effect transistors (FETs) and solar cells [4–6]. In addition, it is an ideal candidate for potential applications in biomedical, chemical and industrial processes enhanced or enabled by the use of new graphene materials [7–9]. These applications of graphene requires a critical understanding of its thermal properties which are key to design future graphene based nano-electronic devices. In addition, the increasing demand to manufacture graphene based nano-components for applications in aerospace, defense and electronics is one of the major incentives to study the thermal properties of graphene.

Numerous studies have been undertaken to predict the thermal properties of graphene sheet. Cai et al. [10] deployed laser heating and monitoring of Raman G-peak to determine the room temperature thermal conductivity of graphene sheet

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synthesized using chemical vapor deposition (CVD) process. They found that graphene possess extremely high thermal conductivity of about 2500 W/mK at room temperature and decreases to about 1400 W/mK at 500 K. Similarly, Ghosh et al. [11] reported the thermal conductivity of graphene as grown across trenches in Si/SiO₂ substrate layer. They found the thermal conductivity of graphene flakes to about 3080–5150 W/mK and possess phonon mean free path of 775 nm near room temperature. Theoretical studies have also been conducted to estimate the thermal conductivity of graphene sheets. Evans et al. [12] made use of equilibrium molecular dynamics (MD) to study the thermal conductivity of graphene sheet with smooth and rough edges. They found that the thermal conductivity is highest for graphene sheet with smooth edges, whereas it is equal for graphene sheet with armchair and zigzag edges. Zhong et al. [13] made use of non-equilibrium MD simulation to deduce the thermal conductivity of graphene sheets. They found that the room-temperature thermal conductivity decays monotonically with the number of the layers in graphene. Hao et al. [14] investigated the effect of mono-vacancies and Stone–Thrower–Wales (STW) defects on the thermal properties of graphene sheet using MD simulation. They found that though the defects cause a gradual decrease in the Young's modulus of graphene sheet, their effect on thermal properties is more pronounced. Lan et al. [15] investigated quantum thermal transport properties of graphene sheet using tight-binding techniques. It was found from their analysis that the thermal transport in graphene sheet shows substantial dependence on the width due to edge reconstructions. It is also useful to note that theoretical analysis allows reconstruction of defects, altering of chirality and system size [16,17] to understand the influence of system parameters on the thermal properties of graphene sheet. Hence, MD simulation models can be used as a viable alternative compared to time consuming and expensive experiments for monitoring thermal transport at nanoscale. MD simulation is capable of generating accurate solutions in predicting mechanical and thermal properties of nanoscale system with minimal cost and high rapidity. However, the MD simulation does not provide information on relationship between the input parameters and the generated output. On the other hand, though soft computing techniques (such as GP) can predict the relationship between the input parameters and generated output, they cannot be used to predict system properties in nanoscale materials.

Therefore, there is a need to develop a new embedded simulation approach consisting of MD simulation and soft computing techniques for modeling the material properties of nanoscale materials such as graphene. The new embedded approach combines powerful advantages of accuracy and low cost of MD simulation with the explicit model formulation of the soft computing techniques. These methods require input training data which can be obtained from the MD simulations which is based on a specific geometry and temperature. Considering input data, the soft computing methods can then be able to generate meaningful solutions for the complicated problems [18,19]. Additionally, among the various soft computing methods described above, evolutionary approach, namely, MGGP offers the advantage of a fast and cost-effective explicit formulation of a mathematical model based on multiple variables with no existing analytical models [20,21]. It is to the best of author's knowledge that limited or no work exists on the application of soft computing models on evaluating thermal properties of the nanoscale system. Additionally, the potential future applications of graphene in electronics industry requires a thorough understanding and investigation of various input parameters on the thermal conductivity of graphene sheet.

Therefore, the main purpose of the present study is to investigate the thermal conductivity of graphene sheet. Standard MD simulation approach is employed to investigate the effect of temperature and STW defects on the thermal conductivity of graphene sheet. Data generated from the MD simulations is fed into the paradigm of GP for the formulation of function expressions. The performance of these models is evaluated against the data generated from the MD simulations.

2. MD simulation methodology

This sections explains the MD simulation methodology adopted to determine the thermal conductivity of a single layer graphene sheet (hereafter referred to as graphene). The data generated from the MD simulation is used to provide the input data to the soft computing cluster (Fig. 1) for training and generation of results. Brenner's second generation bond order function (REBO) [22] is used to describe the covalent bonding of the carbon atoms in graphene. The REBO potential is ideal for simulating a system consisting of large number of hydrocarbon atoms while maintaining the accuracies of semi-empirical and *ab initio* techniques [23–25]. The REBO potential is described mathematically as,

$$E_{REBO} = V_R(r_{ij}) - b_{ij}V_A(r_{ij}) \quad (1)$$

where the repulsive and attractive pair terms are given by V_R and V_A respectively. The b_{ij} term is used to include the reactive empirical bond order between the atoms.

The simulation model consists of graphene sheet of dimensions measuring approximately 10 Å long and 21 Å wide. The thermal conductivity is measured for two types of chirality, viz. armchair and zigzag. The graphene sheet is equilibrated at first to release any residual stresses by achieving thermal equilibrium in an NVT ensemble. In NVT ensemble, the potential energy of the system is minimized by keeping the number of atoms (N), volume (V) and temperature (T) of the system to be constant. The temperature stability of the system is achieved by employing the Nose–Hoover thermostat [26,27]. During equilibration, the system is allowed to relax at every 1000 time steps such that the atoms attain the favorable minimum energy positions. The system is equilibrated for 200,000 time steps with each time step equivalent to 1 fs are used in the simulation.

In order to study the influence of defects on thermal transport in graphene sheet, we manually reconstructed STW defects [28] in the geometry of graphene sheet. STW defect is type of crystallographic defect in graphene sheet. A typical STW defect

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