Proceedings of the

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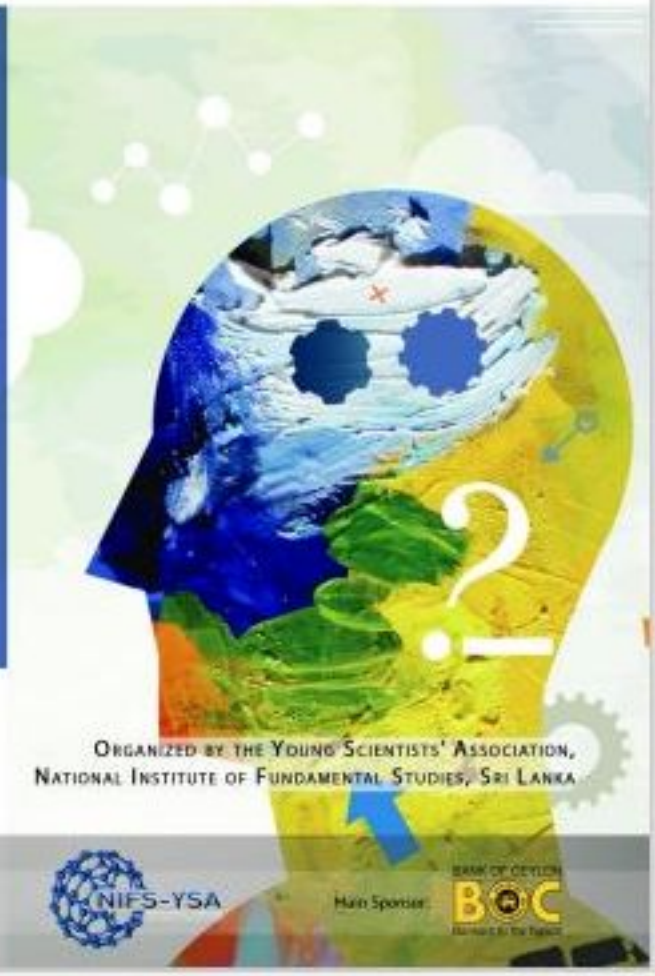

NCMR 2020
08th October 2020

Organized by the Young Scientists' Association,
National Institute of Fundamental Studies, Sri Lanka

NIFS

NIFS-YSA

Main Sponsor: BOC

ISSN 2756-9063
Proceedings of the National Conference on Multidisciplinary Research-2020
Young Scientists' Association, National Institute of Fundamental Studies, Sri Lanka
October 08, 2020

Combined molecular dynamics – representative volume element modeling of thermal conduction of graphene monolayer deposited on an amorphous silicon dioxide substrate

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Due to their higher electrical and thermal conductivity properties, graphene and graphene-based materials have largely attracted the attention in the field of materials science. The electrical conductivity of suspended monolayer graphene is up to 240 000 Ω^{-1} m^{-1} and thermal conductivity is between 2100-5300 W m^{-1} K^{-1} which is one of the highest values known so far. The remarkable electrical and thermal properties make graphene a perfect material to be used in electrical devices. However, graphene has limitations when it is to be used as a thermoelectric material due to its high thermal conductivity. In an attempt to reduce its thermal conductivity, we have experimentally deposited a few layers of graphene onto a Si/SiO_2 substrate using a thermal evaporation technique. To the best of our knowledge, this methodology was used for the first time in the world. The reduction of graphene's thermal conductivity, when supported on a substrate, was first predicted by Klemens et al. The experimental investigations on this phenomenon was previously reported by Seol and Prasher. In this work, we developed an analytical model using a Representative Volume Element (RVE) approach to explain the heat transport of supported graphene. To calculate the in-plane thermal conductivity and inter-layer thermal conductivity between the graphene and SiO_2 layers and to validate the analytical model, we performed extensive molecular dynamics (MD) simulations. The graphene-SiO_2 system was built and analyzed using Visual Molecular Dynamics (VMD) v1.9, and MD calculations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code. The results from the MD simulations were in excellent agreement with the analytical model, which indicates that our analytical model can be used to accurately describe the heat transport in supported-graphene.

Keywords: *graphene, thermal conductivity, molecular dynamics, computational*