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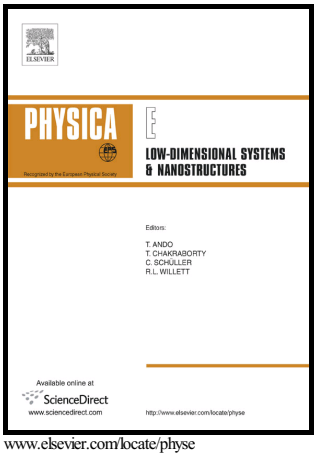


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# The effect of temperature, defect and strain rate on the mechanical property of multi-layer graphene : coarse-grained molecular dynamics study

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**Abstract**

In this work, we investigate the effect of temperature, defect, and strain rate on the mechanical properties of multi-layer graphene using coarse-grained molecular dynamics (CGMD) simulations. The simulation results reveal that the mechanical properties of multi-layer graphene tend to be less sensitive to temperature as the layer increases, but they are sensitive to the distribution and coverage of Stone-Wales (SW) defects. For the same number of defect, there is less decline in the fracture stress and Young's modulus of graphene when the defects have a regular distribution, in contrast to random distribution. In addition, Young's modulus is less influenced by temperature and defect, compared to fracture stress. Both the fracture stress and Young's modulus have little dependence on strain rate.

**Keywords:** coarse-grained, uniaxial tension, multi-layer graphene, mechanical properties



## 1. Introduction:

Graphene, composed of covalently bonded carbon atoms, with the honeycomb lattice, has attracted significant research interest due to its outstanding characteristics in optics, electricity and mechanics since its discovery [1]. Such superior performance enables it to be used in a wide range of areas, such as composite material [2], super capacitor [3], as well as the electrochemical sensing [4]. Based on atomic force microscope nanoindentation, Single-layer graphene has been investigated and proved to be the strongest material with the high mechanical stiffness and