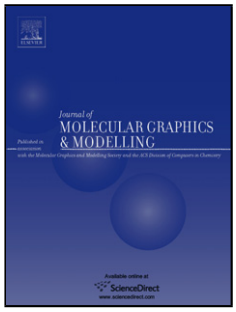

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Temperature distribution in graphene doped with nitrogen and graphene with grain boundary

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Graphene doped with nitrogen exhibits unique properties different than perfect graphene. The temperature distribution in nitrogen-doped graphene (N-graphene) and in the graphene with grain boundary is investigated using molecular dynamics simulations. The temperature distribution in nitrogen-doped graphene nanoribbon, containing two types of grain boundaries, was found to be sensitive to the number of dopants and grain boundary. We also found that there is a remarkable temperature gap in the temperature profile of N-graphene nanoribbon-containing a grain boundary. For any doping ratio N/C we found that the nitrogen atoms enhance roughness of N-graphene and decrease thermal conductivity.

Keywords: Graphene, Nitrogen-doped graphene, Grain boundaries, Temperature distribution, Thermal fluctuation, Molecular dynamics simulation.

I. INTRODUCTION

Graphene has attracted much attention since its discovery in 2004 [1]. It has unique physical properties which are very promising for development of nanotechnology [2–9]. Graphene has the largest thermal conductivity among other materials, i.e. about $1000\,\mathrm{Wm^{-1}}K^{-1}$, making it a good candidate for thermal management in nanoelectronic applications [10]. Graphene can be considered as an isotropic 2D-material that allows using membrane theory for describing its thermomechanical properties. By using raman scattering measurements and Fourier's law of heat conduction, the temperature distribution in a graphene membrane can be determined [11] which results in a thermal conductivity of about $630\,Wm^{-1}K^{-1}$. The chemical doping is an effective way to change the properties of matter [12]. Nitrogen atom contains five valence electrons and an atomic size comparable to that of carbon atoms, therefore, it can be considered an excellent element for chemical doping in graphene [13, 14]. N-graphene has been used in field-effect transistors and lithium ion batteries and also, as an electro catalyst for fuel cell application [15]. Shaoet al. [16] has reported that N-graphene electro chemical activity is much more than that of graphene. Nitrogen doping has been applied to change the structural and electrical properties of carbon nanotubes [17–23]. Because of the higher electronegativity of the nitrogen atoms, it leads to a significant charge redistribution as well as influencing the spin density. These unique properties suggest that the N-graphene becomes chemically more active than graphene. Recently, we studied the structure and polarization effects in the N-graphene [24]. We found that the graphene layer is mechanically weaker when doped with nitrogen, resulting in a decrease of the Young's modulus and the breaking stress. The formation energy also increases as a function of the number of dopants, which results in a decrease in the stability of the nitrogen-doped graphene. Here, we extend our previous work [25] and investigate the effects of nitrogen atoms on the temperature distribution in N-graphene. We also investigate the radial distribution of temperature in a N-graphene with grain boundary using molecular dynamics (MD) simulations. The The linear temperature gradient contained a gap going from the right side to the left side of the grain boundary line. Moreover, we found that the height variations of N-graphene is significantly affected by the presence of nitrogen dopants.

II. THE MODEL

In Fig. 1(a) we show a perfect graphene doped with four nitrogen atoms. The nitrogen atoms were randomly replaced by the carbon atoms. We did not allow two nitrogen atoms (red dots) to be in the vicinity of each other. This structure has been realized experimentally [19]. In Figs. 1, graphene (a), defected graphene having three type of grain boundary in the midline, i.e. large-angle grain-boundary (LAGB)I shown in (b), LAGBII (c) [27], and double LAGBI (d) which are two parallel LAGBI line in opposite direction separated by 5Å. In fact, a grain boundary is a periodic array of 5-7 topological defects located in the y-direction with angle θ. Here, we studied two kinds of LAGB described by θ=21.8^o (LAGBI) and θ=32.2^o (LAGBII) in the literature [26, 27]. In Fig. 2 we illustrate the N-graphene (without grain boundary) system used for studying the temperature profile in the radial direction. Different colors represent different regions used to calculate the temperature gradient. This model is helpful to elucidate experimental results [11].