Investigate the effect of temperature, length, width, and thickness of substrate on thermal conductivity of graphene copper nanocomposites

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The novel thermal conductivity of graphene-copper (GN/Cu) nanocomposites, which include thermal transport of phonons and electrons, has attracted tremendous attention for the development of next-generation nanoelectronic and optoelectronic device applications. To study the effect of temperature, length, width, and substrate thickness on thermal conductivity, Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software has been taken to perform molecular dynamics (MD) simulation. The Green Kubo methods with Embedded Atom Method (EAM), Reactive Empirical Bond Order (REBO), andLenard-Jones (L-J) potentials were used to analyze interactions of atoms. First of all, the thermal conductivity of copper and graphene at 300k temperature has been observed. The thermal conductivity of (GN, GN/Cu (10 0), GN/Cu (110), and GN/Cu (111)) was observed by a wide range of temperature (300K to 1000K). Thermal conductivities of GN, GN/Cu (1 0 0), GN/Cu (1 1 0) and GN/Cu (1 1 1) at 300k were obtained as 1500 $Wm^{-1}K^{-1}$,1204$Wm^{-1}K^{-1}$,1005 $Wm^{-1}K^{-1}$,897 $Wm^{-1}K^{-1}$ respectively. It was witnessed that the thermal conductivity of GN/Cu (1 0 0), GN/Cu (1 1 0), and GN/Cu (1 1 1) decreased by 80.26%, 67%, 59.8% as compared to graphene by changing temperature. It was also observed that thermal conductivity of GN/Cu (1 0 0), GN/Cu (1 1 0), and GN/Cu (1 1 1) decreased by 231.30%, 221.01%, 231.26% with the change in thickness of the substrate. It was calculated that thermal conductivity of GN/Cu (1 0 0), GN/Cu (1 1 0), GN/Cu (1 1 1) increased by 290.7%, 323.98%, 523.1% within length variation from 7nm to 11.0nm.It was also calculated that thermal conductivity of GN/Cu (1 0 0), GN/Cu (1 1 0), GN/Cu (1 1 1) increased by 290.7%, 323.98%, 523.1% within width variation from 0.8 nm to 2.0 nm. Finally, it was concluded that thermal conductivity increased with the increase of length as well as width. It was investigated that the above-mentioned parameters significantly improve the thermal conductivity of GN/Cu (111), which is beneficial for high-performance nanoelectronic and optoelectronic devices include solar cells.

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1. Introduction

In recent years, graphene copper nanocomposites gain numerous attractions in the world of two-dimensional materials. These are attractive materials for various technological applications due to extraordinary large values of thermal conductivity. The recent progress in science and technology enables the size reduction of electronic devices up to the nano level. The heat dissipation in devices has become a crucial problem with the size reduction. The locally generated heat (overheating) is not easily removed from materials and always remains an issue for thermal applications. Consequently, a large number of studies have been completed in the literature for the solution of the overheating problem since it affects badly the thermal properties of materials. Since graphene copper nanocomposites gain attraction in the world of two-dimensional materials and nanoelectronic field [1]. These are striking materials for different technological applications based

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on greater thermal conductivity over high temperatures in developing thermoelectric materials, thermal barrier coatings, and heat dissipation in high power electronics. The ultra-thin layered structure exceptionality of GN/Cu nanocomposites has been considered essential for different applications as mentioned above [2].

The prime mechanism of heat transportation inside graphene is based on phonon vibrations. The contribution of heat transport in copper depends on electrons. The most interesting issues are perceptive of the thermal properties of graphene with metal interactions [3]. The effect of the interface between graphene and metal is also important in optoelectronic devices, integrated electronics, and thermal management applications. It has been observed that the graphene-metal interface significantly affects thermal as well as structural properties due to interactions between carbon and metal atoms [4-5]. However, it has been observed that free electrons in metals contribute significantly to underestimate thermal conductivity [6].

The novel thermal conductivity of graphene copper nanocomposites had been extensively investigated by MD simulation with the Green Kubo method. However, the experimental approach can provide measurements directly related to novel thermal conductivity but due to the limited capability of nanoscale temperature, experimental cost suffers great challenges for investigations. It is very difficult to predict interfacial kinetic properties without the true knowledge of thermal conductivity by using EAM potential [7]. Since, a large number of researchers have considered Cu adhered to a single layer of graphene (SLG) for calculation of energy, stress, structure, and interaction strength through the geometry of atoms [8]. It has been observed that the thermal conductivity for graphene copper nanocomposites due to acoustic phonons($330Wm^{-1}K^{-1}$) and for longitudinal phonons ($654Wm^{-1}K^{-1}$) respectively [9]. Graphene copper interface has a much stronger effect on thermal conductivity which decreases up to ($525Wm^{-1}K^{-1}$), due to strong open d-orbital couplings [10-13]. It has been observed that length and width may affect thermal conductivity extensively toward the improvement of thermal properties of graphene copper nanomaterial [14-15].In recent work; a theoretical approach has been used to obtain thermal conductivity of graphene copper nanocomposites.

However, it has been observed that temperature is one of the main factors which considerably affect the thermal conductivity of GN/Cu nanocomposites [16-17].The GN/Cu nanocomposites thermal conductivity decreases ($510Wm^{-1}K^{-1}$) to ($440Wm^{-1}K^{-1}$) due to interface conductance between copper and graphene which improves the thermal performance of graphene copper nanocomposites [18-20]. A comprehensive understanding of the thermal interface between graphene and metal is essential for next-generation energy storage and electronic devices [21-24]. The thermal interface between graphene-Au and graphene-Cu affects thermal conductivity significantly and the interface is designed for different pairs which are normally from one to three orders of magnitude [25]. Metals are considered superior thermal conductive and high thermal expansion coefficient materials in many applications. However, thermal conductivity improvement in graphene metal composites generally depends on position along with an arrangement of graphene as well as metal besides affecting thermal properties [26-29]. On the other hand, it was demonstrated that thermal conductivity enhances due to atomistic simulations, the geometry of the material especially by changing the temperature [30-33].

In this study, it was observed that the effect of temperature, length, width as well as thickness of substrate improved the novel thermal conductivity of graphene copper nanocomposites. In recent times, graphene copper nanocomposites have been proposed for many applications due to their extraordinary values of thermal conductivity through the above-mentioned factors. This study is valuable in nano-scale control electronics and thermal transport engineering management applications. The outcomes of the current work provide a broad understanding of various factors that affect noticeably the thermal conductivity of the GN/Cu nanocomposites.

2. Theory and Simulation

2.1. Interatomic Molecular Dynamics Potentials

The interatomic MD potentials are used for the transport of acoustic phonons in graphene and electrons in metal through MD simulations for graphene along with copper atoms interactions entirely. Despite this, thermal conductivity accuracy can improve with the use of suitable interatomic potential which easily represents the interaction of atoms. Different kinds of potentials are used for various interactions during the whole simulation. In this study, we have performed computation for Cu-Cu interactions through Embedded Atom Method (EAM) potential and its Equation is

$$E = \sum F_i(\sigma_{ij}) + \frac{1}{2}\sum_i \sum_j (\emptyset)_{ij}(R)_{ij} \qquad (1)$$

Here,$F_i(\sigma_{ij})$ is the electron density embedded energy. The term$(\emptyset)_{ij}(R)_{ij}$ is the repulsive interactions between core atoms. One must be familiar with the host atoms, embedded energy, and repulsive force through EAM potential in MD simulations. For accurate interaction between graphene and copper atoms, Lenard-Jones (L-J) potential was employed. The L-J potential used for the computation of non-bonded interaction energy for the reason of better accuracy in relating bond order and its Equation is given as

$$V_{lj} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad (2)$$

Hereσ represents the finite distance when the interparticle potential is zero. The termε is used for potential well depth. The distance between two atoms is r. The material characteristics depend on values of εand σ which describe adhesiveness and lubrication properties. The potential parameters are given as

$$\varepsilon_{Cu-C=0.02578ev} \qquad (3)$$

$$\sigma_{Cu-C=3.0825\text{Å}} \qquad (4)$$

The value of ε used in the range 0.01-0.05ev. In this study, Reactive Empirical Bond Order (REBO) potential was employed for heat transport within graphene to give a better narrative regarding thermal conductivity.

2.2. Equilibrium Molecular Dynamics (EMD) Simulation; The Green -Kubo Method

The system remains constantly within the linear response regime during EMD simulation. The transport coefficients were computed through the Green-Kubo method. Thermal conductivity can be interrelated throughout equilibrium current-current autocorrelation function using Green-Kubo expression and its Equation is given as

$$\mathrm{K} = \mathrm{V}/\mathrm{K_B}\,\mathrm{T}^2 \int_0^t J(t)J(0) > dt \qquad (5)$$

where T is system temperature and K_B used for Boltzmann constant. Here, tis the correlation time and V fora volume of a system equal to the product of area and Vander walls thickness (3.4 Å). Meanwhile, t=m$\nabla T$is the correlation time where∇T = time step in MD simulation. The total no of time steps is (N). The terms heat current (J) and$J(t)J(0) >$ used for heat current autocorrelation function (HCACF) which can be computed as

$$J = \frac{1}{V}\sum_i eiVi - \sum_i SiVi \qquad (6)$$

Here $\boldsymbol{e_iV_i}$ is total kinetic and potential energy. The term $\boldsymbol{S_iV_i}$ is a stress tensor. The Green -Kubo method has beenused to converge accurately HCACF. It has been found that heat flow fluctuates directly around zero in a system of particles. The thermal conductivity of GN/Cu nanocomposites has been investigated by using the linear response theorem and heat fluctuation-

dissipation. Resultantly, it has been concluded that Green-Kubo is the easiest and accurate method for thermal conductivity calculation.

2.3. Basics of Heat Transport in Graphene Copper Nanocomposites and Thermal Conductivity

Thermal conductivity is the measurement of the transport of acoustic phonons in graphene as well as electrons in copper. Thermal conductivity is an important property of materials that describes the relation of a temperature gradient with heat flux, J through Fourier's law. Thermal conductivity can be found by Fourier's law and its relation is$J = -K\nabla T$, where heat flux (J), thermal conductivity (k) along temperature gradient (∇T). The thermal conductivity depends on phonons in graphene and electrons in copper at the same time as

$$K = Kp + Ke \tag{7}$$

where$Kp$and Ke are the thermal conductivity of phonons and electrons. As within graphene phonons are dominant whereas electrons dominant inside copper for heat transfer here in the graphene copper nanocomposites. Thermal conductivity significantly changes owing to modification of phonon energies collectively with phonon scattering and phonon electrons scatterings. The acoustic phonon interactions through electrons in copper reduced thermal conductivity appropriate to spatial confinement. Moreover, thermal conductivity depends on size which changes phonons' electrons interactions at what time the system changes from 2D to 3D. Hence phonons boundary scatterings within graphene extensively affect thermal conductivity. In recent years, Pop and co-workers bring to being lower thermal conductivity within graphene-based systems. In this research work, we have discussed significant changes in thermal conductivity suitable to orientations of copper and by varying copper layers in addition to variation in temperature, length as well as the width of nanocomposites.

2.4. Model and Simulation Details

The model for thermal conductivity observation of graphene and GN/Cu nanocomposites is represented in figure 1. For instance, SLG laminated on Cu substrate in various orientations as Cu (1 0 0), Cu (1 1 0), and Cu (1 1 1) as shown in figure 1. In the recent study, interactions between Cu-Cu atoms in the MD model have been described with the use of EAM potential developed by Mishin*et al.* [34]. This accurate potential reproduces all lattice parameters such as elastic constants, thermal expansion, phonon frequencies, and cohesive energy as well as many significant properties of Cu. This unique potential predicted melting temperature (1327 K) of Copper which is concurrence to the experimental value of (1357 K) [35].In recent calculations, the temperature is considered in the wide range of 300k to 1000k. It was investigated that the long-wavelength phonons contribute dominantly to thermal transportation even at the lowest temperature as the Debye temperature. Despite this, the temperature considered near 343 K which is the Copper Debye temperature [36].The simulation block is cubic and periodic boundary conditions applied in all directions to avoid the effect of fixed walls throughout simulations. In the present work, a stable configuration of hexagonal one atom thick GN layer on the Cu substrate was carried out with EMD simulation [37]. The lattice constant of copper and SLG have been taken as (3.615Å), 2.46Å. MD simulation is employed by using LAMMPS code for thermal conductivity of graphene Cu nanocomposites [38]. The inter-atomic forces can be described by REBO, EAM, and L-J potentials with periodic boundary conditions [39-40]. The Muller Plathe which is implemented in the LAMMPS software required both heat gradients along with heat flux to estimate thermal conductivity. The correlation length and sample interval are taken as 1000 and 10 correspondingly. The structures are first minimized using the conjugate gradient method [41]. To obtain a steady-state, the Noose Hoover thermostat is used for no fluctuations time and makes the temperature average around. Visualization of the atomic structures has been seen with the visual molecular dynamics (VMD) program [42]. The whole data analyzed averaged with the MD simulations at zero pressure by isothermal-isobaric (NPT), canonical (NVT) as well as the micro-canonical

(NVE) ensemble. The ensemble NPT was employed for a time of 0.182 fs. After stabilizing the whole system, the NVT ensemble is changed to an NVE ensemble for better calculations [43-45].

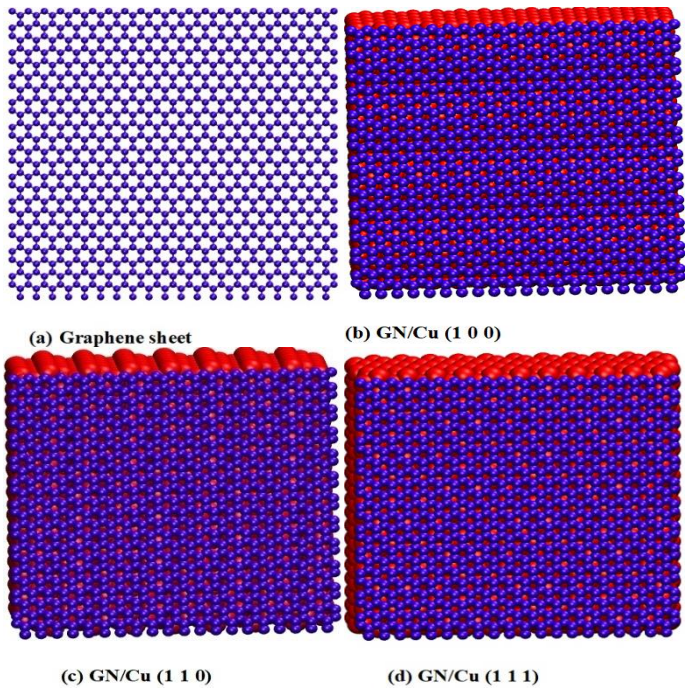

Fig.1. Schematic presentation of simulation model (a) Graphene sheet (b) GN/Cu (1 0 0) (c) GN/Cu (1 1 0) and GN/Cu (1 1 1).

Thermal conductivity of copper has been obtained with unit cell dimensions (40Å, 40Å, 15Å) for a time step of 0.001ps at 300 K. Therefore, temperature varies from 300 K to 1000 K to obtain thermal conductivity of GN, GN/Cu (100), GN/Cu (110), and GN/Cu (111). Since, a square graphene sheet with unit cell dimensions (50Å, 50Å) has been taken for a time step of 0.182fs. Hence, the thermal conductivity of the GN/Cu nanocomposites has been calculated with unit cell dimensions (50Å, 50Å, 5Å) for a time step of 0.182fs. Since, the thermal conductivity of GN/Cu (100), GN/Cu (110), and GN/Cu (111) nanocomposites have been observed with the variation in length from (7.0 nm to 11.0 nm) with a fixed width of 10nm to check the effect of length. At the same time, the width is also varied from (0.8nm to 2.0nm) with a fixed length of 10nm. Resultantly, the effect of substrate thickness on thermal conductivity has been observed by the variation of some layers (1 to 5) of copper respectively.

3. Results and Discussion

Thermal conductivity of GN/Cu nanocomposites was observed due to phonons in graphene and free electrons in copper for heat transportation. For instance, SLG laminated on Cu substrate in various orientations as Cu (100), Cu (110), and Cu (111) as shown in figure 1. For this purpose, a wide range of temperatures 300 K to 1000 K was employed. The particular range of temperature, width, and length has been taken which affect significantly phonon scatterings. Moreover, the number of copper layers varied from 1 to 5 for estimation ofbetter thermal conductivity. The obtained results of the present work have been agreed with measured data in the literature. This support could be applied for other materials which pave the path for thermal conductivity enhancement of high-temperature materials. While the closer observation of this study reveals that these main factors significantly affect heat conduction in graphene copper nanocomposites.

3.1. Temperature Dependence of Thermal Conductivity

The thermal conductivity is a function of temperature within a wide range of temperatures (300 K to 1000 K) as shown in figure 2.The thermal conductivity decreased with the rise of temperature as was observed in the literature. The simulation of thermal conductivity of GN, GN/Cu (100), GN/Cu (110), and GN/Cu (111) showed that the bonding strength causes a reduction in the thermal conductivity. Moreover, the bonding strength restricts the movement of atoms at a larger temperature which creates an obstacle for phonon transportation. Figure 2 depicts the decreasing trend of thermal conductivity for GN, GN/Cu (100), GN/Cu (110), and GN/Cu (111) with the rise of temperature. It was observed that thermal conductivity in pure composite lattice structure decreased due to phonon-phonon scatterings [46]. Initially, copper and graphene thermal conductivity has been observed at 300K. As reported in the literature, the thermal conductivities of copper and graphene were observed as ($385 Wm^{-1}K^{-1}$) and ($991 Wm^{-1}K^{-1}$) respectively. The variation of temperature plays an important role in thermal conductivity reduction due to phonons- phonons and phonons- electrons interactions. The physics of thermal transportation of phonons, as well as electrons, is complicated in GN/Cu nanocomposites. The heat conduction takes place due to acoustic phonons in graphene and electrons in copper. However, the interactions of phonons with electrons change thermal conductivity with the rise of temperature. Many factors affect these interactions due to the disorder of the composite system and temperature is one of the main factors. Since it was reported that high-frequency phonons increased by increasing temperature. The phonons umklapp scatterings also increases which reduces the thermal conductivity. As it has been examined that in crystalline materials due to strong umklapp scattering the thermal conductivity decreases with the rise of temperature. In this study, a square graphene sheet of (50Å, 50Å) has been taken at 300k temperature with REBO potential to estimate thermal conductivity. The main reason is a finite size, as well as a mean free path which affects thermal conductivity with the rise of temperature. Hence, a very sharp gradient of temperature during this process possibly changes as shown in figure 2. It can be seen that transportation of heat inside GN/Cu nanocomposites not only diffusive and examined by temperature gradient. The temperature dependence of thermal conductivity is essential commencing both physics as well as applications points of view. The number of short-wavelength phonons increases by increasing temperature. The umklapp scattering increases by increasing the number of high-frequency phonons which reduced thermal conductivity. A large scattering of phonons along with electrons plays an important role in thermal conductivity. At lower temperatures, thermal conductivity varies with the inverse of temperature but it deviates at a larger temperature [47]. Besides the interaction of acoustic phonons with optical phonons at larger temperature also affect thermal conductivity [48].

The umklapp process at a lower temperature is inactive and umklapp scattering becomes significant at higher temperature [49]. Resultantly, it was observed that thermal conductivity decreased by increasing temperature. As shown in figure 2 thermal conductivity of graphene is 1500 $Wm^{-1}K^{-1}$ which is higher as compared to GN/Cu (1 0 0), GN/Cu (1 1 0), and GN/Cu (1 1 1). The thermal conductivity dependence employing temperature agrees reasonably well through experimental data at a wide range of (300k to 1000K) temperature. In recent work, the thermal conductivities of GN, GN/Cu (1 0 0), GN/Cu (1 1 0) and GN/Cu (1 1 1) at 300K were obtained as 1500 $Wm^{-1}K^{-1}$,1204$Wm^{-1}K^{-1}$,1005 $Wm^{-1}K^{-1}$,897 $Wm^{-1}K^{-1}$ respectively. The results of our study follow a similar trend of thermal conductivity variation with an increase of temperature since reported by Mehdizadeh et al [50] 2500 $Wm^{-1}K^{-1}$ and 1700 $Wm^{-1}K^{-1}$ at 300 and 400K. It was calculated that the thermal conductivity of GN/Cu (1 0 0), GN/Cu (1 1 0), and GN/Cu (1 1 1) decreased 80.26%, 67%, 59.8% as compared to graphene. The outcomes of the recent study showed that the thermal conductivity of GN/Cu (1 1 1) was lowest as compared to GN/Cu (1 0 0) and GN/Cu (1 1 0).

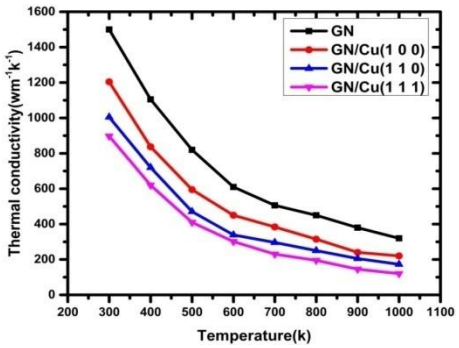

Fig.2.Thermal conductivity of GN (black), GN/Cu (1 0 0) (red), GN/Cu (1 1 0) (blue) and GN/Cu (1 1 1) (pink) as a function of temperature.

Table 1.Thermal conductivity with temperature variation.

Temperature (K)	GN ($Wm^{-1}K^{-1}$)	GN/Cu (1 0 0) ($Wm^{-1}K^{-1}$)	GN/Cu (1 1 0) ($Wm^{-1}K^{-1}$)	GN/Cu (1 1 1) ($Wm^{-1}K^{-1}$)
300K	1500	1204	1005	897
400K	1105	837	720	620
500K	820	595	471	410
600K	610	450	339	301
700K	506	384	296	230
800K	450	315	250	195
900K	380	240	205	145
1000K	320	220	173	120

3.2. Length Dependence of Thermal Conductivity

Fig 3 depicts the variation in length from (7.0nm to 11.0nm) of graphene-copper nanocomposites structures. The linear extrapolation procedure was used to investigate thermal conductivity predictions for various lengths. Thermal conductivities of GN/Cu (100), GN/Cu (110), and GN/Cu (111) as a function of variation in length from (7.0nm to 11.0nm) with a fixed width of 1nm increases with increases in length as shown in figure 4. The main reason for the scattering process was the mean free path of phonon. Phonons behave as dominant for thermal conduction inside graphene. The electrons within the copper were dominant for thermal conduction. The bulk phonons mean free path may considerably change thermal conductivity at room temperature. It has been observed that phonon-phonon interaction increases the number of phonons by increasing length.

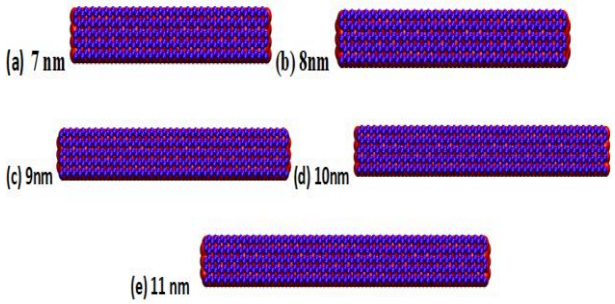

Fig. 3. Schematic atomic structures of GN/Cu nanocomposites with variation in length from 7 nm to 11 nm with a fixed width of 10 nm.

This causes a faster decay of thermal conductivity. Another factor that affects the thermal transport in graphene metal composite is flexural phonons in graphene and electrons in copper.The flexural phonons in this context in graphene are responsible for the source of heat carriers and prevent deviation in thermal conductivity. However, lower frequency acoustic flexural phonons are required for accurate thermal conductivity. On the other hand, Nika et al observed that out-of-plane acoustic phonons did not involve in heat transportation [51]. Meanwhile, Sonavane et al considered that flexural phonons play an important role in the thermal conductivity of graphene by changing length which is in agreement with our research [52].On the other hand with the involvement of REBO potential, the thermal conductivity increases by increasing the length. So in this context, thermal conductivity dependence on length is mainly due to the phonons boundary scattering process. The variation in the length of composite controls sharply phonons mean free path. The acoustic phonons of longer wavelength are available in favor of larger length and more heat transfer through the composite. The long-wavelength weakly scattered phonons in graphene scattered in three Umklaap processes. By comparing with the length of composite toward phonons mean free path, the Umklaap processes become negligible, and next to the edge, phonons collision becomes an important scattering process. Consequently, when the length becomes smaller the edge scattering becomes stronger. The edge scattering becomes weaker at a larger length which decreases the thermal conductivity. The transportation of heat in graphene occurs due to more acoustic phonons. Therefore, long-wavelength phonons are responsible for this transportation of heat. Since the edge scattering phonon prevents heat transport with smaller lengths due to the mean free path of phonons [53].The highest value of thermal conductivity has been observed at 300k with a fixed width of 10nm of GN/Cu (1 0 0), GN/Cu (1 1 0), GN/Cu (1 1 1) are 3623 $Wm^{-1}K^{-1}$, 3363$Wm^{-1}K^{-1}$ and 3102 Wm^{-1} K^{-1} respectively. The thermal conductivity of GN/Cu (1 0 0) increases from 1246 $Wm^{-1}k^{-1}$ to 3623 Wm^{-1} K^{-1} with length variation. The thermal conductivity of GN/Cu (1 1 0) increases from 1038 Wm^{-1} K^{-1} to 3363 Wm^{-1} K^{-1} whereas GN/Cu (1 1 1) increases from 593 Wm^{-1} K^{-1} to 3102 Wm^{-1} K^{-1} respectively. It has been calculated from above-mentioned results that thermal conductivity of GN/Cu (1 0 0), GN/Cu (1 1 0), GN/Cu (1 1 1) increases 290.7%, 323.98%, 523.1%. It has investigated from present outcomes that thermal conductivity of GN/Cu (1 1 1) increases greater within length variation from 7 nm to 11.0 nm which is better for nanoelectronic devices where heat dissipations occur quickly.

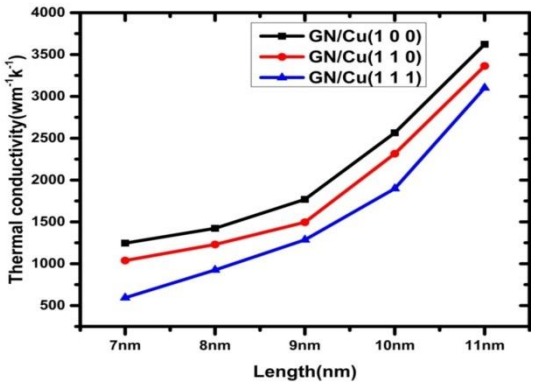

Fig. 4. Thermal conductivity variation of GN/Cu (1 0 0) (black), GN/Cu (1 1 0) (red) and GN/Cu (1 1 1) (blue) as a function of length at 300k temperature with fixed width 10nm.

Table 2. Thermal conductivity with length variation at fixed width 10 nm.

Length (nm)	GN/Cu (1 0 0) ($Wm^{-1}K^{-1}$)	GN/Cu (1 1 0) ($Wm^{-1}K^{-1}$)	GN/Cu (1 1 1) ($Wm^{-1}K^{-1}$)
7	1246	1038	593
8	1423	1230	925
9	1769	1495	1285
10	2565	2315	1898
11	3623	3363	3102

3.3. Width Dependence of Thermal Conductivity

It has been shown from figure 6 the effect of width on thermal conductivity. It can be seen that by increasing width thermal conductivity increases. Since the effect of boundary scattering becomes weaker by increasing width while the effect of edge localized phonon decreases. Hence, the thermal conductivity increases. Besides, it has been observed that the lamination of graphene on the copper substrate reduced phonon scattering. Consequently, It has been predicted that the thermal conductivity of GN/Cu (111) composite smaller than GN/Cu (100) and GN/Cu (110) respectively. It is perceptible that by increasing width, thermal conductivity also increases. Thermal conductivity monotonically increases with the mentioned width range from figure 5. The effect of electrons in the metal, the edge localized phonons, phonons umklaap, along with boundary scattering in graphene drastically change composite thermal conductivity. The boundary scattering increases in graphene which increases the number of phonons. The electrons in metals and phonons increase the interaction in graphene significantly change thermal conductivity by increasing width. Since larger phonons are activated this creates phonons umklaap effect.

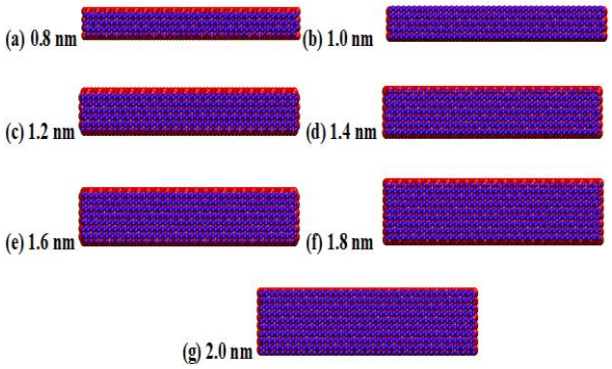

Fig. 5. Schematic atomic structures of GN/Cu composites with variation in width from 0.8nm to 2.0nm with fixed length 10nm.

It has been shown from figure 6 that GN/Cu nanocomposites in favor of widths increasing, thermal conductivity monotonically increases at greater width and rate ceases due to boundary scattering along with Umklapp scattering [54]. Therefore, for narrower composites effect of boundary scattering become dominant as compared to umklapp scattering. By increasing width, a reduction in edge localized phonon also occurs. It has been observed that for wider composite, the impact of boundary scattering enervated, and the number of phonons increases. The umklapp scattering becomes higher which speedily increases the number of phonons [55]. Moreover, figure 6 shows that by increasing width, the edge scattering increases which is a favorable condition for thermal transportation inside GN/Cu nanocomposites. It has been observed that the thermal conductivity at 0.8nm of width with a fixed length of 10nm for GN/Cu (1 0 0), GN/Cu (1 1 0), and

GN/Cu (1 1 1) are 1387$Wm^{-1}K^{-1}$, 933Wm^{-1} $K^{-1,}$ and 660Wm^{-1} K^{-1}respectively. It has been also investigated that thermal conductivity at 2.0 nm of width for GN/Cu (1 0 0), GN/Cu (1 1 0) and GN/Cu (1 1 1) are 10823Wm^{-1} K^{-1}, 8280Wm^{-1} $K^{-1,}$ and 6125 Wm^{-1} K^{-1} respectively. It has been calculated from above-mentioned results that thermal conductivity of GN/Cu (1 0 0), GN/Cu (1 1 0), and GN/Cu (1 1 1) increases 780.31%, 887.45%, 928.03% within width variation from 0.8 nm to 2.0 nm. The obtained results show that the thermal conductivity of GN/Cu (1 1 1) is greater as compared to GN/Cu (1 0 0) and GN/Cu (1 1 0).

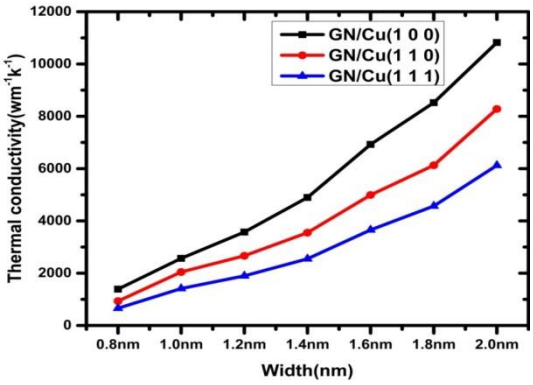

Fig. 6. Thermal conductivity variation of GN/Cu (1 0 0) (black), GN/Cu (1 1 0) (red) and GN/Cu (1 11) (blue) as a function of width at 300k temperature with fixed length 10nm.

Table 3. Thermal conductivity with width variation at fixed length 10 nm.

Width (nm)	**GN/Cu (1 0 0) ($Wm^{-1}K^{-1}$)**	**GN/Cu (1 1 0) ($Wm^{-1}K^{-1}$)**	**GN/Cu (1 1 1) ($Wm^{-1}K^{-1}$)**
0.8	1387	933	660
1.0	2565	2043	1412
1.2	3573	2665	1898
1.4	4896	3549	2548
1.6	6925	4992	3654
1.8	8523	6128	4570
2.0	10823	8280	6125

3.4. Thermal Conductivity Dependence on Substrate Thickness

Figure 7 shows the variation inthe number of copper layers. The schematic structures of copper layers have been represented with red colors at the bottom. The hexagonal structure of graphene is represented with a violet color. It has been shown in figure 8 that the thickness of the substrate significantly affects thermal conductivity. Figure 8 shows the variation in thermal conductivity of GN, GN/Cu (1 0 0), GN/Cu (1 1 0), and GN/Cu (1 1 1) with the different number of layers. It has been found that the thermal conductivity decreases by increasing the number of layers. Thermal conductivity of single layer of GN/Cu (1 0 0), GN/Cu (1 1 0), and GN/Cu (1 1 1) at 300K has been observed as 3173 $Wm^{-1}K^{-1}$, 2818 Wm^{-1} $K^{-1}$and 2660 Wm^{-1} K^{-1}respectively. Thermal conductivity for five layers of copper for GN/Cu (1 0 0), GN/Cu (1 1 0), and GN/Cu (1 1 1) at 300K have been observed as 1372 Wm^{-1} K^{-1}, 1275 Wm^{-1} $K^{-1}$and 1150 Wm^{-1} K^{-1}respectively. It was calculated from recent results that thermal conductivity of GN/Cu (1 0 0), GN/Cu (1 1 0), and GN/Cu (1 1 1) decreased by 231.30%, 221.01%, 231.26% respectively.

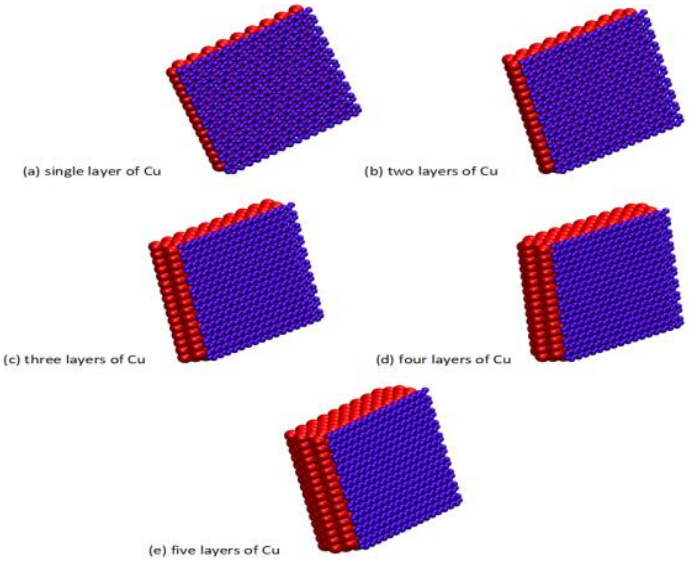

Fig. 7. Graphene copper nanocomposites with copper layers at the bottom (a)single layer of Cu (b)two layers of Cu (c)three layers of Cu(d)four layers of Cu (e)five layers of Cu with red color and graphene with violet color on top of the copper.

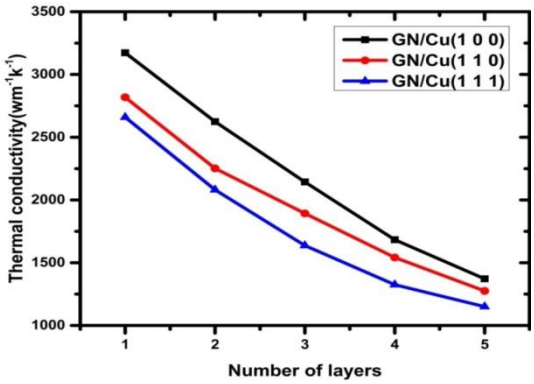

Fig. 8. Thermal conductivity variation of GN/Cu (1 0 0), GN/Cu (1 1 0), and GN/Cu (1 1 1) as a function of the number of copper layers from 1 to 5.

Table 4. Thermal conductivity with the number of copper layers variation.

Number of copper layers	GN/Cu (1 0 0) ($Wm^{-1}K^{-1}$)	GN/Cu (1 1 0) ($Wm^{-1}K^{-1}$)	GN/Cu (1 1 1) ($Wm^{-1}K^{-1}$)
1	3173	2818	2660
2	2624	2225	2081
3	2144	1893	1637
4	1683	1542	1325
5	1372	1275	1150

4. Conclusion

Heat transport characteristics in graphene copper nanocomposites have been studied to analyze the impact of copper orientations, temperature, length, width, and thickness of substrate on thermal conductivity. Therefore, it has been explored thermal conductivity decreases with increasing temperature and substrate thickness. The thermal conductivity increases by increasing

length and width due to the weakening of phonon boundary scattering in wider composites. The above-mentioned results show that GN/Cu (111) has better thermal conductivity. These results provide important guidance to improve thermal conductivity which might be useful in energy storage devices, nano electronics, and optoelectronic devices include solar cells in the future to solve the problem of heat dissipation.

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