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Research Article

Defects Induced Variations in Thermal and Mechanical Properties of Graphene-Silver (C-Ag) Nanocomposites: A Molecular Dynamics Simulation

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Abstract

A Single Layered Graphene (Gr)sheet exhibit extraordinary mechanical and thermal properties. Understanding the GN/Ag contact is crucial for analyzing the impact on dislocation movements and how it influences thermo-mechanical performance. In this work we have create defects in graphene sheet by removing single or multiple atoms. Three orientations of Ag ((1 0 0), (1 1 0), and (1 1 1)) and different defects concentrations in monolayer graphene were selected to study the impact of temperature and stress during heating, dislocation nucleation can be caused by edges in graphene in addition to the interface. The melting temperatures of defective GN/Ag (1 0 0), GN/Ag (1 1 0), and GN/Ag (1 1 1) were measured at 300K.Additionally, all samples underwent ultimate tensile stress. The stress of defective GN/Ag (1 0 0), defective GN/Ag (1 1 0), and defective GN/Ag (1 1 1) was determined. For (100) orientation was 16.0GPa, for (110) orientation is 12.01GPa, for (111) orientation was 14.2GPa. So, we can see here ultimate tensile stress is better in (100) orientation then other orientations. According to the data provided, GN/Ag nanocomposites show promise for use in heat management applications.

Keywords: *Graphene, Heating, Dislocation, Nucleation*

1. Introduction

Graphene metal nanocomposites are receiving significant interest because to their interfaces and dislocations, since they are being developed for applications requiring extremely high strength in the car and aerospace sector. Furthermore, combining graphene with silver enhances both mechanical strength and design functionality, making it valuable for a wide range of technical applications. Researchers have created graphene metal nanocomposites with different levels of increased hardness and strength. Graphene is a distinctive two-dimensional material composed of sp^2 hybridized carbon atoms arranged in a honeycomb crystal lattice. It possesses exceptional properties such as a large surface area of 2630 m2, high visibility to light and maximum thermal conductivity of around 5000 $Wm^{-1}K^{-1}$outstanding mechanical strength (young's modules ~1.1TPa).

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Silver is used in industrial gear, whereas graphene is a layer that is just one atom thick. These two are top competitors because of their strong thermo-mechanical performance, valued in both the aerospace and car industries. Graphene metal nanocomposites are often produced commercially to enhance the thermo-mechanical properties of materials used in the automotive and aerospace industries, resulting in stronger cars and aircraft components.

Nanocomposites are used in the production of several components of passenger aircraft, such doors, spoilers, fairings, and elevators, to enhance fuel economy and decrease weight. It is essential to use lightweight, cost-effective, and durable nanocomposites. Nanocomposites are preferred over polymer composites for their lightweight properties, thermal stability up to high temperatures (1000C°), and very high mechanical strength.

Material (such as nickel, iron, aluminum, gold, copper, titanium) are group of metallic elements on the other hand also nonmetallic element (such as carbon, nitrogen, oxygen) in relative to small amount[1].

Metals are hard but malleable, shiny and little in color. These materials have high density and good conductor of electricity [2]. Pure metals are commercially 99% pure minimum. These Metals have not been alloyed with other metallic elements[3]. Pure metal contains atoms that are only one type of metallic element. Some Examples of pure metals are Zinc, copper, aluminum, Gold etc. Alkali metals are the metals that having low melting point and these metals be a part of IA group in periodic table. For example, Cs, Rb , K. Alkaline-earth metal is belong to group IIA group from periodic table[4]. These metals oxides fabricate by alkaline earths that is why they are called Alkaline earth metals. For example beryllium (Be), magnesium (Mg), calcium (Ca), strontium (Sr), barium (Ba), and radium (Ra) are Alkaline earth metals[5-8]. Graphite was discovered by K.W. Scheele in 1779[9]. He was a Swedish scientist. Graph good conductor of electricity and heat. It is also called black lead or plumage. It is crystalline shape of carbon in hexagonal system[10-12]. Graphite mostly used in nuclear reactors, electric motors, lamps, batteries, pencils, lubricants, crucibles, polishes, and foundry facings etc. Due to its high conductivity, it is used in electronic products[13-15]. It is brittle and soft in form so it can be used as powder form for different tasks. Graphene is a two-dimensional material discovered by A. K Geim and K. S Novoselov in 2004[16].A perfect graphene having 2D crystalline covalently bonded atoms, has high thermal and mechanical properties and also having high electric properties[17]. Graphene(Gr) also be the good material in the field of application in flexible electronics[18-20]. Graphene having zero band gap in the field of electronics band structure [21]. Graphene have one sheet of atoms arranged as hexagonal Lattice. Graphene (Gr) having better thermal, mechanical and other properties. Graphene (Gr), having a perfect two-dimensional crystal structure, and extraordinary electrical, thermal and mechanical properties[22-26]. However, during the growth process, lattice defects will certainly can be produced [27-31]. In general, defects in graphene can be categorized into different types [32-34]. In the presence of defect like that point defects and by changing the square width of defects in graphene sheet are change the various properties [35]. These various defects in graphene sheet the composite with silver could remarkably affect the mechanical and thermal properties[36-38]. In the last few years, work on properties of defected graphene sheet broadly [39]. For example Ng et al. investigated the changes in the thermal conductivity of graphene for two different chirality cases and densities of STW defects using Molecular Dynamics (MD) simulations [40]. Experimentally in fabricated graphene having different types of defects. We know that defects in graphene sheet effects the thermal and mechanical properties [41]. There are different types of defects present in graphene sheet like that single vacancy defect, multiple vacancy defect, line defect. Stone-wales defect, substitution of atoms and grain boundaries [42-45]. So as to every kind of defect effect the different properties of graphene sheet [46-48]. The main objective of this paper is to make the simulation model of defective graphene/silver nan-composite and check the thermal and tensile properties at different temperature and different percentage of defect concentration[49]. In this work, we examine the effects of different defect concentration (like that 2%, 15 % and 30%) of randomly distributed defects like that point defect[50-52]. The main thing we should be noted that accuracy of molecular dynamics simulation is dependent on different types of interatomic potential. We used periodic boundary condition in our modeling for removing the effect of boundary atoms[53]. In other situation we used shrink boundary condition to count the effect of boundary atoms. Many peoples have investigate the thermal and mechanical properties of pristine and defected graphene sheet by different method. But my purpose is to investigate thermal and mechanical properties of defected graphene and silver nanocomposite. In this work, we used non equilibrium molecular dynamic (NEMD) method for analyzing the thermal conductivity and mechanical properties. Remarkably, we noticed that results of different orientation (like 100,110,111) by increasing the square width of vacancy is very close[54]. We observed that increasing the length or width also effects the thermal conductivity at room temperature[55]. By performing Uni-axial tensile stress on the material, we investigate the mechanical properties of the material[56]. It was observed that stress increases linearly with strain till it reach proportionality limit, in which stress is directly proportional to the strain known as elastic limit. In elastic limit if we remove applied stress, material will return to its original shape[57]. After elastic limit, increased stress permanently changed the material and did not gain its initial shape after the removal of applied stress. This region is known as plasticity. It was observed that different defect concentration gives different results of thermal conductivity. Furthermore, as in overall trend, we observed that material gives better mechanical behavior at (100) orientation[58-62]. The latest effort aims to investigate enhancing the thermo-mechanical performance of graphene copper nanocomposites for use in the car sector and aerospace applications. Graphene metal nanocomposites have garnered significant interest in the car and aerospace industries due to their impact on material structure, mechanical strength, and design possibilities.

Simulation model

Molecular dynamic simulation is a method in which we can explore the movement of atoms by using computer simulation method. In this method molecules an atoms are granted to interact to each other for a fix period of time. MD simulation has been extensively used for modeling with atomic scale resolutions. Molecular dynamic simulation tool invented by Rahman and

Alder and Wainwright in 1950s and early 1960s. In 1970s due to advancement in computer field this method also be upgraded and use at atomic level for this study of properties of materials. Molecular dynamic simulation is computational method to get information about two or more than two interacting particles by applying some specific tools or method. Molecular dynamic simulation system is very useful to handle many body systems. In this method we can examine properties of any material. In molecular dynamic simulation atoms are look like balls. Molecular dynamic simulation is economical method to get valuable result and study the properties of materials. In molecular dynamic simulation we applied some technique to get valuable result. In which 1st of all we make ready a specific model for a specific task. In a classical method, newton 2nd equation of motion is simple equation for many body systems. Newton 2nd equation is:

$$F_i = m_i a_i \quad (1)$$

Here, we can see that` F` is a force between any two atoms or molecules and `m` is the mass of atoms or molecule and `a` is acceleration. We also know that this equation not useful for associating properties of an electrons. In simple words this 2nd equation is not useful for very small size particles. We can overcome this problem by using Schrödinger equation of motion in Quantum mechanics. Molecular dynamic simulation is mostly used to investigate the mechanical, thermal and optical properties. In Molecular dynamics simulation position will be change by movement of atoms in some specific direction. In vast number of atoms each atom exerts a force on other atom. When these are close to each other then they exert a strong force to each other due to strong interaction of atoms. Conjugate gradient method is the one of the basic technique for energy minimization. In this work Nose Hover Thermostat is temperature controlling method. When simulation process occurring then this method rashly the velocities of atoms for controlling the temperature. In this molecular dynamics simulations, the Green-Kubo formula is used to compute transport coefficients. Thermal conductivity is related to auto-correlation function that can expressed by Green-Kubo formula,

$$K = {}^{1}/_{3}\, K_B\, T^2 V \int_o^{\infty} < J(t).J(0) > dt \quad (2)$$

In this simulation process we have used different types of potential like that Lenard-jones (LJ) potential for the attraction of C-Ag atoms and other is Airebo potential which is used interaction of carbon atoms. We used Velocity-Varlet's method is used to calculate the velocities of atoms. In this whole simulation process systems run to 50, 0000 time steps and each time step is 0.182 fs. So this system is equilibrated at the required temperature in the NVT ensemble (constant number of atoms, volume and temperature). For the mechanical properties the single time step is set to 0.182 fs and whole system is run for 600000 time steps. The mechanical properties of defective Gr/Ag (100), (110) and (111) we applied uni-axial tensile stress along x-axis at strain rate 5Giga per second.

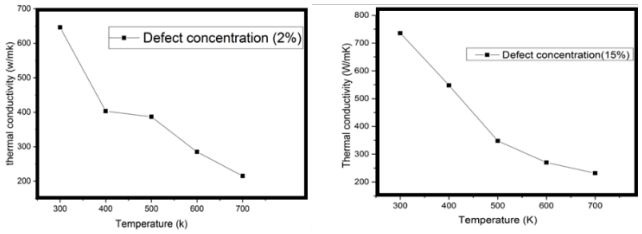


Fig.1 Effects of 2% & 15% defects concentration in graphene sheet and investigate thermal conductivity of graphene/silver nanocomposite

At both defect concentration thermal conductivity is decreases by increasing the temperature. Defect density is defined as number of defects are divided by number concentration. We know that according to the classical theory of lattice, thermal conductivity is proportional to mean free path of phonon scattering, that is given as

$$\lambda = {}^{1}/_{3}\, CVl \quad (3)$$

Here, we can see in this equation, C is specific heat capacity, V is group velocity in the form of sound wave in solid and l is the mean free path of pure graphene can be calculate by phonon-phonon scattering.

Now in the existence of defects the mean free path is changed into,

$${}^{1}/_{l_{eff}} = {}^{1}/_{l_{ph-ph}}\, {}^{1}/_{l_{def-ph}} \quad (4)$$

Now according to this equation we can that $l_{ph\text{-}ph}$ shows that phonon- phonon scattering and $l_{def\text{-}ph}$ shows that the length scattering in the presence of defects. According the both equation (3) and (4) thermal conductivity of defective graphene/silver composite satisfied this relation.

$${}^{1}/_{\lambda} \propto {}^{1}/_{l_{ph-ph}} - {}^{1}/_{l_{def-ph}} \quad (5)$$

Now, we can see in eq.5 defective graphene/silver acquires less thermal conductivity due to phonon scattering generated by the defects. Moreover, the humiliation of thermal conductivity depends on defects density.

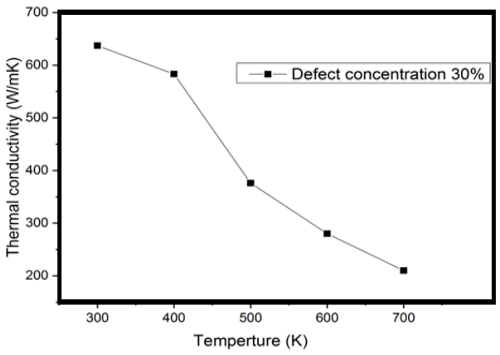


Fig.2 Effect on thermal conductivity by changing the defects concentration 30%

So by increasing the defect density, more phonon-defect scattering appear and $l_{def\text{-}ph}$ decreases. As the end of, according to eq.5 thermal conductivity is decreases. In 15% defect concentration in a graphene(GN) sheet also change the thermal conductivity of composite with silver. We can see in **Fig.1** the thermal conductivity is decreasing by in increasing the temperature in 15% defect concentration. Furthermore in 30% defects concentration thermal conductivity is also decrease by increasing temperature we can see this phenomena in **Fig.2.**

So the thermal conductivity (k) of defective Graphene/silver (Gr/Ag) (100), (110) and (111) nanocomposites is calculated by increasing width of all orientation at 300K keeping length 1 nm as shown in figure 3 and 4.The defect concentration is 1 % in a graphene sheet. The thermal conductivity (k) is increased by increasing width, because number of atoms also increases and more phonons are available for thermal conductivity (k) as shown in figure.

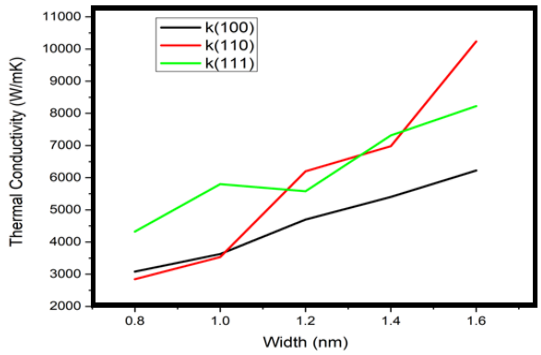


Fig.3 Comparison Graph between three orientations to check the thermal conductivity by changing the width

Thermal conductivity (k) of Defective Graphene/silver (Gr/Ag) (100), (110) and (111) nano composites is also calculated by increasing length of all nanocomposites at 300K keeping width 1 nm as shown in **Fig.5** and **Fig.6**.

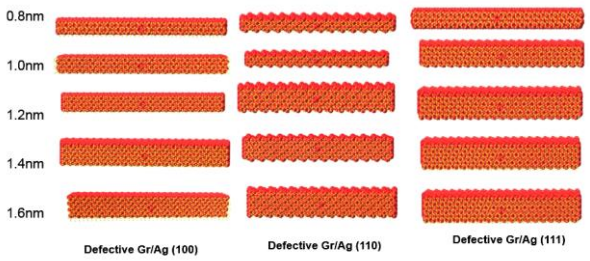


Fig.4 Model of width of Defective graphene/silver nanocomposite

The thermal conductivity (k) is increased because as length increased, number of atoms also increased and more phonons are available for thermal conductivity (k) as shown in figure 6 but we can see that result of thermal conductivity (111) orientation shows better result than other orientations. Defects concentration is 1 % during this whole process to find the thermal conductivity by changing length.

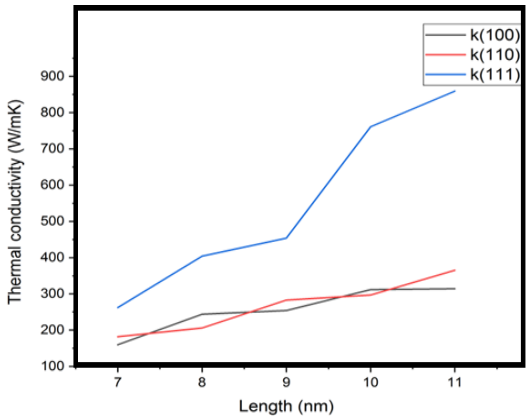


Fig.5 Comparison Graph between three orientations to check the thermal conductivity by changing the length

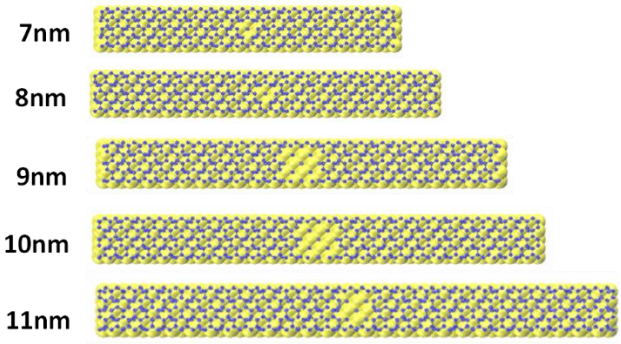
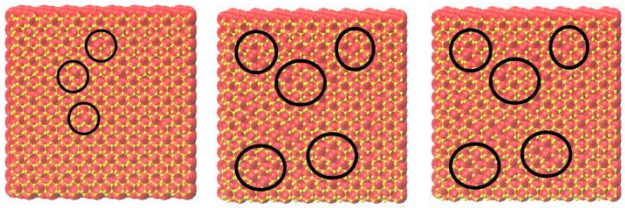


Fig.6 Model of length of Defective graphene/silver nanocomposite.

Mechanical behavior of defective GN/Ag Nanocomposite

In our research work, we use Silver (Ag) as a substrate on which we placed Graphene (Gr) layer with square width of defects to investigate the mechanical properties. The plane orientation of Silver (Ag) that are (111), (110) and (100). Dimension of composite is 40Å x 40Å x 19.3Å. The periodic boundary conditions are applied in all direction. The lattice constant of Silver (Ag) and atomic mass of Silver (Ag) are 4.079Å and 107.868 gram/mole respectively. In this simulation, tensile rate of silver (Ag) was controlled by applying strain to find out in-plane mechanical properties. The time-step is set to 1fs. Initially temperature is increased from 10K to 300K and then thermalized at 300K by using isothermal-isobaric (NPT) ensemble for 10000 steps. Tensile rate for simulation box is controlled by strain rate of about $5x10^{9}ps^{-1}$. The loading process takes 600000 steps. Silver (Ag) and defective Graphene (Gr) atoms are shown in different color below, red color for Silver (Ag) slab and yellow graphene sheet with defects as shown in figure 8.



Defective GN/Ag 100 (b) Defective GN/Ag 110 (c Defective GN/Ag 111)

Fig.7 There are there different orientation like (100),(110),(111) model of defective graphene(GN)/ silver(Ag) nanocomposite

Result and discussion

We have investigated the mechanical properties of defective Graphene/Silver (Gr/Ag) (100), (110) and (111) nanocomposites by applying uni-axial tensile stress by using MD simulations. The molecular dynamics MD simulations is technique that are used for this model to elaborate the uni-axial stretching result in the presence of Graphene (Gr) sheet on the surface of Silver (Ag).

In **Fig.8**, we can see that by increasing the stress rate , the deformation also increased. Initially stress increased linearly with strain till it reach proportionality limit, in which stress is directly proportional to the strain known as elastic limit. In elastic limit if we removed applied stress, composite obtained its original shape. After elastic limit, increased stress permanently deformed the composite and did not gain its initial geometry after the removal of applied stress. This region is known as plasticity. After that composite reached at ultimate tensile stress UTS (maximum stress that material can bear). Further increased in stress smashed the composite permanently. Defective Graphene/Silver (Gr/Ag) (100), (110) and (111) have ultimate tensile strength UTS about 16.04 GPa, 12.01 GPa and 14.2 Gpa respectively as shown in figures 9, 10 and 11. Then material starts to deform after that limit. From figure 11 It is cleared that when applied uni-axial tensile stress increased, material started to deformed from middle side and then atoms start to move far apart to each other. After that Silver (Ag) slab permanently deform. Atomic crystallography is different of both materials that is why there exist lattice mismatch at interface. There also exist elastic distortion and chemical interaction energy between atoms. Therefore, strength of nanocomposite is improved. During stretching process, initially atoms of Graphene (Gr) sheet are dislocated and then this deformation transfers towards the silver (Ag) substrate. During stretching of composite, in the case of defective Graphene/silver (Gr/Ag) (100) and (110) cavity is formed at the middle of composite. In case of Gr/Ag (111) nanocomposite, there exist necking phenomenon at the middle side of composite as shown in figure 11. As dislocations are further increased to certain value then this tiny hole starts to enlarge in size smoothly and extends completely the whole silver slab. So, material is deformed permanently. Deforming process of defective Graphene/silver (Gr/Ag) nanocomposite is complicated than pure silver (Ag). Because these composites have different cracking stages like Graphene (Gr) sheet cracking, metal cracking and finally interface cracking during applied uni-axial tensile stress process. Ductility of Graphene (Gr) sheet and flexibility of carbon atoms in Graphene (Gr) sheet is not beneficial. So, Graphene (Gr) deformed first. We can see that the comparison of three orientations the UTS of 100 orientation is better than other two orientations.

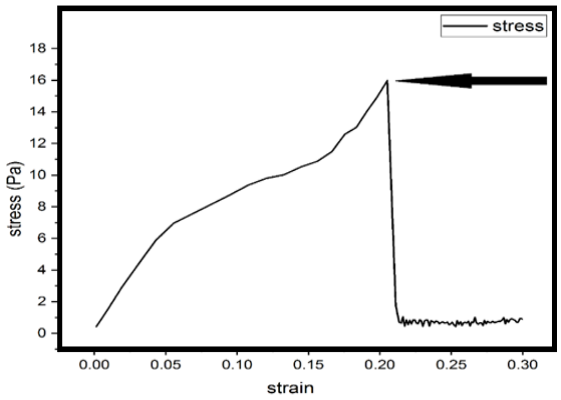


Fig. 9 Stress-strain curve for (100) Orientation

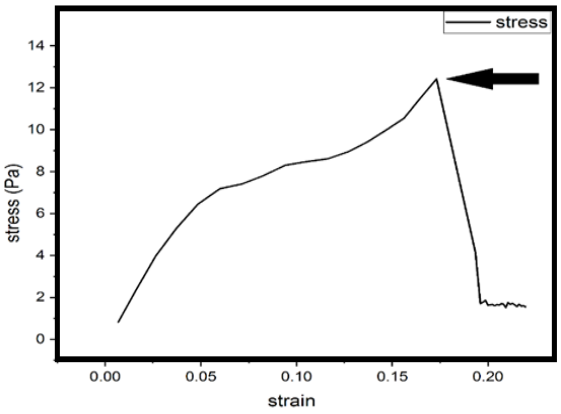


Fig.10.Stress-strain curve for (110) Orientation

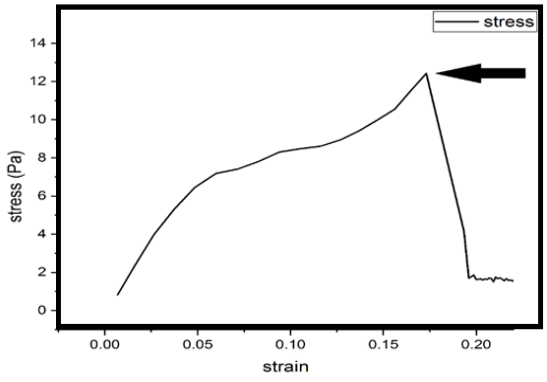


Fig.11 Stress-strain curve for (111) Orientation

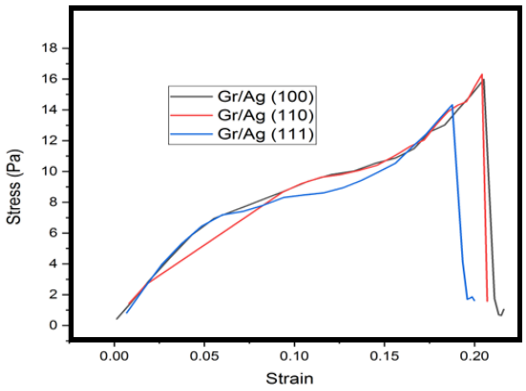


Fig.12 Comparison of Stress-strain curves for all orientation

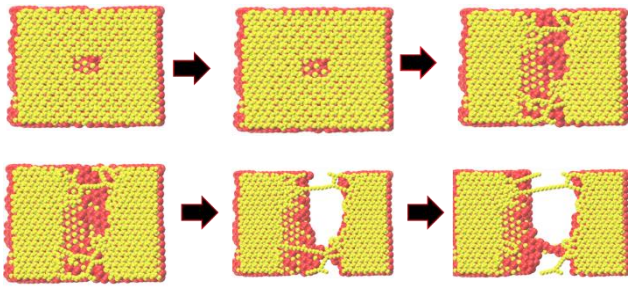


Fig.13 Deformation behavior of Defective Gr/Ag nanocomposite along horizontal direction

Conclusion

Thermal conductivity can be calculated by using Molecular dynamics simulation of defective graphene/silver nanocomposite. There are three different orientations like that (100), (110) and (111) of silver matrix is used with graphene sheet with defects using different types of potential is used. Before to find the thermal conductivity of composite we have made a defective graphene sheet by removing a single atom or multiple atom and also change the defects concentration in a graphene sheet. To analyze that interaction between silver atoms and carbon atoms of graphene sheet defects. We use EAM potential and AIREBO potential respectively. For the interaction among the silver and graphene atoms we use LJ potential. The thermal conductivity depends upon different factor like length, width and temperature difference. Thermal conductivity of graphene sheet increases with the increase of length. The increase in width of graphene sheet increases the thermal conductivity. The change in temperature causes good effect in thermal conductivity. In this work, we examine the effects of different defect concentration (like that 2%, 15 % and 30%) of randomly distributed defects like that point defect. At 2% defect concentration thermal conductivity is decreases by increasing the temperature and in 15% and 30% defect concentration thermal conductivity also decreases by increasing the temperature. Defect density is defined as number of defects are divided by number of atoms in pure graphene The main thing we should be noted that accuracy of molecular dynamics simulation is dependent on different types of interatomic potential.The work offers insights into the melting and deformation process in graphene-Silver nanocomposites, which might improve the efficiency of producing and advancing graphene-metal nanocomposites for applications in automotive and aerospace industries. At To analyze the mechanical properties by MD simulations, we investigate the effect of graphene sheet with defect on silver substrate with different orientation of silver metal like (100), (110) and (111). It is also noticed that the presence of graphene sheet on silver substrate increases the ultimate tensile strength. Ultimate tensile strength of defective graphene/silver (100) is 16.0GPa and Ultimate tensile strength of defective graphene/silver (110) is 12.01GPa. Ultimate tensile strength of defective graphene/silver (111) is 14.2GPa. So we can see here ultimate tensile stress is better in (110) orientation then other orientations.In short, we can say that our result shows the extraordinary mechanical properties of that composite. So, this composite can be used for the practical purposes in different fields.

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