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A study to overcome the electrical behavior limitations of defective Cu/graphene composites using molecular dynamics

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ABSTRACT: In the process of handling and bonding copper (Cu) and graphene, defects inevitably occur. Therefore, in order to use the Cu/graphene composite as an electronic device, it is important to evaluate the effectiveness of such defects. In this paper, microscopic physical phenomena were analyzed by molecular dynamics simulation(MDS).
As a result, it was found that certain defects in the stress distribution occurred depending on the location.

I. INTRODUCTION

New materials that exceed the existing performance, such as graphene, are found, and in the process of manufacturing and processing these new materials, micro-nano technology has reached a level that can be operated in the range of molecules and atoms. Based on these technologies, new materials are contributing to various fields such as medical devices, aerospace, displays, and high-performance portable devices.[1-5]

For example, Apple, launched in 2007, attempted to change from the existing mobile phone market, which was centered on calls, to the information delivery-oriented smartphone market through the iPhone. Since then, wearable devices such as smart watches and electronic device industries such as Z-flips, curved monitors, rollable TVs, and tablet PCs have developed. The development of the industry has led to a demand for the development of new materials with high transparency, bottom resistance, and unique characteristics that can be used for flexible displays that can be folded or bent beyond the performance of existing displays.[6-8]

Graphene is a material that began to gain attention as a representative future new material during this period. This is because graphene is a material with improved performance compared to the existing material while maintaining high strength and flexibility while maintaining the function of the existing display.[9-12]

Graphene is a transparent electrode material with elasticity that preserves electrical properties even with more than 10% deformation on rubber substrates through transfer printing to a substrate where devices can be implemented after separating from synthetic substrates. Graphene, a two-dimensional material, has a very high shape ratio and a specific surface area and is suitable for use in nanocomposites. Graphene with high electrical conductivity, such as metal materials, has excellent elasticity, so it does not lose its electrical conductivity even when bent, It is also excellent in strength. In addition, because it is a material generated from carbon atoms, the cost of raw materials required for production is low, which is an advantage of graphene.[13-17]

For these reasons, graphene has attracted attention as a substitute for ITO with high strength and high electron mobility while reducing material consumption compared to ITO (Indium Tin Oxide, Indium Tin Oxide, hereinafter referred to as 'ITO') which is used as a conventional display material. It maintains performance for a long time as well as a display panel.

Research continued to utilize graphene in a wide range of industrial fields such as battery development, corrosion prevention, electronic circuit boards, medical and health smart wearable devices.

However, in the process of applying graphene as a commercialization stage, technical limitations were revealed in the part of producing it to maintain stability while maintaining the material's inherent excellent physical properties. For example, notches, cracks, scratches, impurities, etc.[18]

Defects inevitably occurred in the process of preparing ultrathin graphene.In addition, it was difficult to stably manufacture large-area graphene in the mechanical peeling method, which was the initial method of manufacturing graphene.

Currently, a lot of commercialization studies have been conducted using CVD (Chemical Vapor

Deposition, Chemical Vapor Deposition, hereinafter referred to as 'CVD') that can produce graphene in a relatively large area, resulting in many meaningful results. This is because the purity is high and in order to be used as a device, graphene must be made into a CVD method that is easy to manufacture a large area.

At this time, graphene is produced with fewer than 10 layers by a general CVD method.

This background is demonstrated by Sherrell et al.'s research that confirmed that one to two layers of graphene produced through CVD methods had conductivity suitable for electrical stimulation, and that Aslanidou et al. showed the best physical properties when the number of layers of graphene combined with electronic devices was created with the number of layers less than 10 through CVD methods.[19,20]

In particular, the smaller the number of layers, the closer to the theoretically proven properties of graphene, but defects due to etching in the process of synthesizing graphene and separating after production inevitably occurred in the manufacturing process using the CVD method.

Various defects occurring in the manufacturing process of graphene deteriorate stability in the stage of using and applying graphene and become an obstacle to the evaluation of physical mechanisms for mechanical and electrical properties, making it impossible to accurately evaluate the safety of products produced with graphene. Therefore, for safe commercialization of graphene, the problem of defects must be solved in advance.

On the other hand, there are currently attempts to solve the problem of safety against such defects using copper in related fields. Copper is a material that has already been commercialized in the manufacturing and processing process, as is generally known. Copper is an optimal material whose safety has been verified due to the easy application of electric/electronic products and the commercialization of the material itself.

Therefore, in the field of graphene-related research, a method of combining and utilizing a metal material such as copper and graphene as a composite material is being studied a lot. In other words, by applying copper and graphene, which are nanomaterials having excellent electrical conductivity, as composite materials to reduce weight and enhance stability when developing mobile electronic devices and electric vehicles, research is being conducted and is attracting attention.

Wu et al.) analyzed the electrochemical properties of metal/graphene composites for use as energy storage devices, and Zhang et al. compared graphene transistors, silicon transistors, and graphene varistors to discuss unique properties for using graphene electronic devices.[21-23]

II. PURPOSE OF RESEARCH

Since graphene is a nanomaterial, molecular dynamics analysis is most suitable to fully realize the microscopic behavioral properties of graphene. And defects affect the performance of copper/graphene composites. Therefore, in this study, copper/graphene composites are stably used as electronic devices, and the basic way to achieve commercial performance improvement using defect characteristics is to be presented. The goal of this study is to evaluate the mechanical and electrical behavior of copper/graphene composites using molecular dynamics.[24-27]

The specific goals of this study are as follows.

First, to evaluate the mechanical properties of tensile analysis, molecular dynamics analysis is used to evaluate the strength of defective copper/graphene composites along zigzag, armchair, and thickness direction.

Second, through electron density analysis, the DOS behavior of copper/graphene composites with or without defects is investigated to evaluate the effect of defects on copper/graphene composites.

To mass-produce copper/graphene composite nanowires, they must be easy to manufacture and safe, and not too thick for commercialization.

In addition, if peeling occurs at the interface, the desired strength and physical properties cannot be obtained when manufacturing a composite material, which causes performance degradation. In order to overcome these limitations, research such as interface and peeling is an essential task for the commercialization of graphene.

Therefore, in accordance with this need, three analysis models were defined that distinguished the thickness of copper. In order to observe the effect and peeling phenomenon on the structural direction of graphene, each analysis model was given individual tensile force according to the analysis conditions. The related results were evaluated from both a mechanical and an electrical perspective. In addition, analysis models were defined and compared for electrical characteristics in consideration of the presence and location of defects. Each analysis model is based on the presence or absence of graphene defects.

For comparison, consider the effect of the presence of defects on the number of layers of copper/graphene.

It is believed that the completed results can be applied through a series of processes to the stability evaluation criteria for defects occurring in the manufacturing process of graphene, which is called the next-generation dream material. On the other hand, since this study performed molecular dynamics evaluation, it is believed that fine phenomenon control will play a pivotal role in the development of smart displays, electrochemical sensors, and high-speed electronic devices.

III. METHODS

MDS analysis for evaluating the mechanical properties of copper/graphene composite materials was performed using LAMMPS, an open source for calculating electronic structures and modeling materials at nanoscale. The copper/graphene composite model used to evaluate the mechanical properties of copper/graphene composite materials in this study was classified into three types according to the copper thickness. Analysis Model I is a sandwich-type laminate structure in which a graphene layer is inserted between the copper layers.

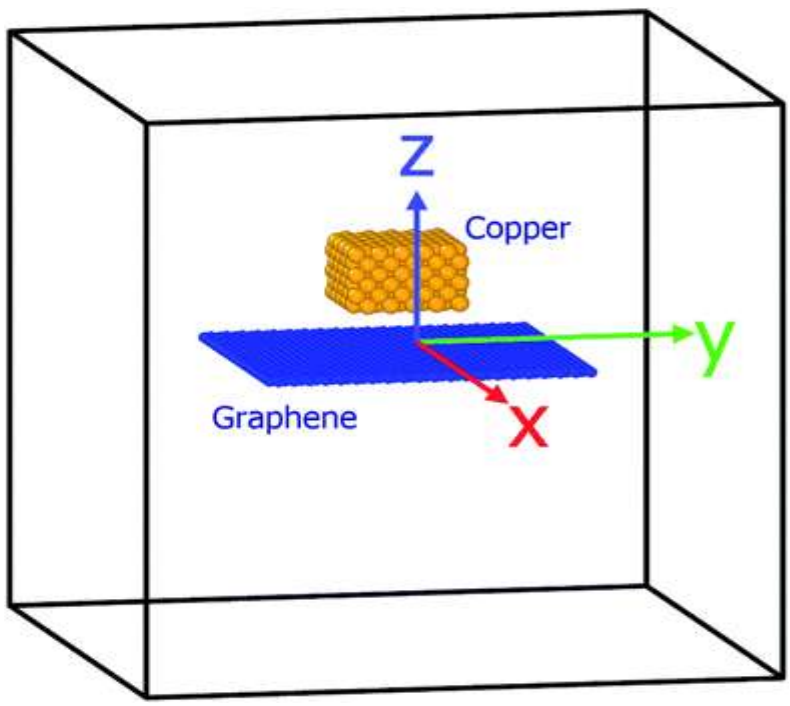
To evaluate the impact of defects on composite materials, break it by dividing it into zigzag direction, armchair direction, and thickness direction. Since the boundary condition of the analysis is a form in which tensile force is applied at both ends based on the x-axis direction, both ends of the x-axis were set as bite points, and the tensile rate was 0.17 nm/ps.

The model for evaluating mechanical properties was modeled using LAMMPS. Analysis model is a stacked shape in the form of a sandwich in which a graphene layer is inserted between copper layers, and the modeling standard of copper/graphene composite is 20.6×11.9×7.4 nm.

In order to evaluate the impact of the box on the composite material, it was divided into four cases according to the analysis conditions, each of which is ND (non-defect, hereinafter referred to as ND) and GD (graphene)

It was named and classified as defective, hereinafter referred to as 'GD', CD (Cu defective, hereinafter referred to as 'CD'), and CT (Cu thickness direction, hereinafter referred to as 'CT').

Finally, the electron density analysis for the evaluation of the electrical properties of copper/graphene composites was performed using Quantum ESPRESSO, an open source for calculating electronic structures and modeling materials at nanoscale. As for the potential condition, Perdue-Burke-Ernzerhof (PBE) was used for all the copper atoms constituting the carbon (C) and copper (Cu) molecules of the graphene molecule.



IV. RESULTS

The analysis results of ND, GD, and CD show rapid stress reduction at both locations until complete destruction in common. The first copper fracture began first, and the stress decreased at a certain stress reduction point, strain ε = 0.1, and then showed a stagnation section. Similar to the metal machining hardening phenomenon, the stress stagnation phenomenon was determined until the graphene was completely broken after the progress of the initial crack.

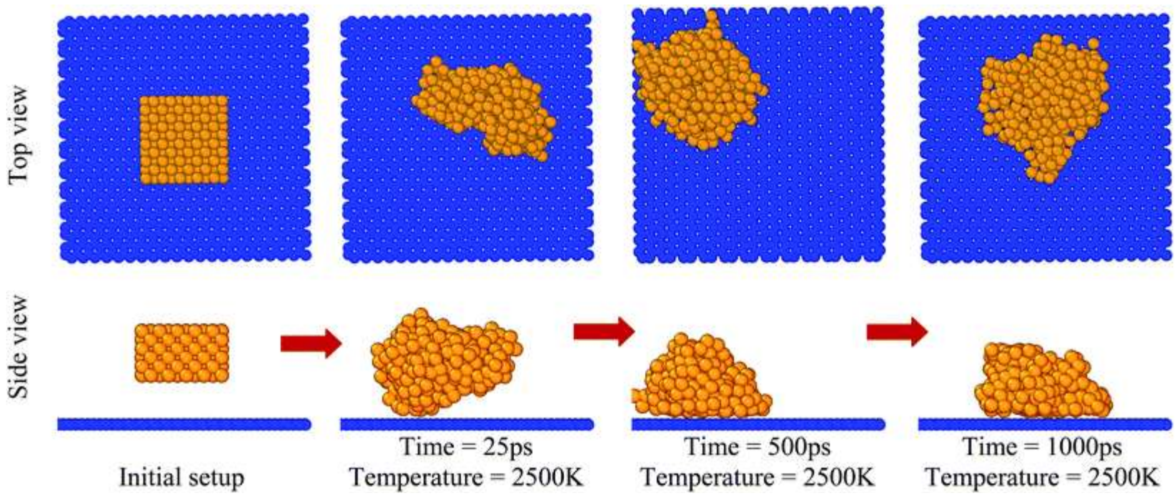
At strain ε = 0.1, the stress value was 19.5 GPa in ND without defects, 19.69 GPa in GD with crack defects in graphene, and 19.43 GPa in CD with crack defects in Cu, which was almost similar. The presence or absence of initial crack defects was found to be almost similar.

It indicates that the crack behavior is not affected until progression. In the case of ND without defects, after entering 14.91 GPa at a strain ε= 0.145, a stress of 16.02 GPa was obtained at a ε = 0.35 and the stress of 14.95 GPa was maintained on average from a strainε = 0.145 to a ε = 0.35, and the final breakage was made. In the case of a CD with copper defects, after entering a strain ε= 14.58 GPa at a strain = 0.14 to 14.58 GPa, a stress of ε = 0.36 to 16.04 GPa was obtained, and the stress of 14.82 GPa was maintained on average between a strain ε= 0.14 and a ε = 0.36, and the final breakage was made. It can be judged that the size set in this study does not contribute to the deterioration of the strength of the entire copper/graphene composite that CD with defect in Cu has a similar stress-strain relationship compared to ND without defect.

However, in the case of GD with defects in graphene, the stress decreased by about 21.7% compared to ND and CD, and after entering 10.83 GPa at a strain ε = 0.155, 10.29 GPa at ε = 0.155, 9.99 GPa at ε = 0.325 and ε = 0.365.

The stress of 10.95 GPa was shown, and the stress of 10.39 GPa was maintained on average in the section from strain ε= 0.145 to ε = 0.325, and then the final fracture was made. This is because defects in graphene affect the strength degradation in copper/graphene composite models.

The reason why the second stress phase point is higher than the initial maximum value is thought to be because the graphene layer was responsible for the stress and supported the model as the copper fracture occurred first.



V. CONCLUSION

This study conducted a mechanical characteristic evaluation and an electronic density analysis evaluation to evaluate the effect of defects, which are risk factors acting in the process of manufacturing copper/graphene composites, on mechanical and electrical behavior. As a result of tensile analysis of graphene in the zigzag direction, as the thickness of copper increased, the breaking strength decreased to 19.7 GPa, 11.5 GPa, and 5.9 GPa, and the strength performance of the graphene/copper composite material deteriorated. In the armchair direction of graphene.

As a result of tensile analysis, as the thickness of copper increased, the breaking strength decreased to 14.9 GPa, 8.9 GPa, and 8.3 GPa, and the strength performance of the graphene/copper composite material deteriorated. When evaluating the mechanical properties of copper/graphene composite materials, copper/graphene composite materials are evaluated.

Pin composites are more vulnerable to tensile force in the armchair direction than zigzag. As a result of tensile analysis in the thickness direction, the relationship between the copper thickness and the copper/graphene composite at the peeling time is weak.

In the copper/graphene composite of the 20.6×11.9×7.4 nm standard, the stress is concentrated in the graphene layer, and graphene was the material that affects the strength leading to the overall composite performance degradation. When a defect occurs in the graphene layer, the lowest fracture strength occurred at 14.35 GPa, making it the most vulnerable to fracture. When a defect occurs in the copper layer, the shape of the defect did not affect the strength, and it affected the strain at which the destruction occurred. It was found that the crack of graphene in the copper/graphene composite affects the strength performance improvement of the entire copper/graphene composite, and the crack in the copper layer affects the degree of deformation of the entire copper/graphene composite.

Two-layer stacked copper/graphene composites in which graphene is stacked on the existing copper layer exhibit stable DOS behavior similar to that of graphene in the entire energy level section, and in certain sections, DOS behavior similar to copper is shown, so both materials are zero.

Compared to the two-layer stacked copper/graphene composite, the four-layer stacked copper/graphene composite with increased thickness increased by about 14.63% or more at the peak point where the DOS value was highest. In particular, the DOS value in the two sections occurred more than twice, improving the electrical performance of the copper/graphene composite against the increase in the thickness of graphene and copper. When a defect is inserted into the two-layer stacked copper/graphene composite, the DOS value decreased by about 22.85% at point A and about 50% at point B compared to the two-layer stacked copper/graphene composite without the defect. That is, on a single graphene, the DOS value decreased by about 22.85% at point A and about 50% at point B.

The defect that occurred reduced the DOS value and degraded the electrical performance.

The above results can be used as a basic method to evaluate defects that may occur during the manufacturing process for the stable design research and development of copper/graphene composites that are indispensable for the commercialization of copper/graphene composites. In the future, in addition to the defect conditions presented in this paper, it can be used as a useful method in consideration of defects that occur during application to products of the desired thickness and size.

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