Thermal Conductivity of Porous Graphene Nanoribbon Implemented in Mass Detection Operations

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ABSTRACT

In this paper, efficiency of defected graphene nano ribbon incorporated with additional nanoparticles on mass detection operations is studied via the Reverse Non Equilibrium Molecular Dynamics (RNEMD) method. Thermal conductivity management of this structure is challenging because of imposed losses in electrical conductivity and any procedure that could manage the thermal conductivity of graphene will be useful. In this paper it is observed that on the mass detection operation, due to the porosity generation in the nano ribbon surface or even creation of external nanoparticles, thermal properties of graphene change considerably. This should be noted in calibration of graphene based mass sensors. In summary, Results show that the graphene’s thermal conductivity would reduce by increasing the concentration of nanoparticles and thermal conductivity of graphene is higher when porosities and impurities are at the edges. This indicates that the location of vacancies and nanoparticles influences the thermal conductivity. For a better thermal management with the help of nanoparticles, with respect to the porosities, addition of nanoparticles decreases the thermal conductivity more.

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Graphene Field Effect Transistors (GFET) is a promising field in the realm of nanoelectronics due to its unique electronic properties and potential applications in various devices. The primary advantage of GFETs is their ability to control the flow of electrons or holes by applying a voltage between the source and drain, making them crucial for future electronic devices. In this section, we will explore the basic principles of GFETs, their fabrication, and their applications.

1. Graphene Field Effect Transistors (GFET)

Graphene, a single layer of carbon atoms arranged in a hexagonal lattice, has garnered significant attention due to its remarkable electronic properties. GFETs exploit these properties by using graphene as the channel material in a field-effect transistor configuration. The electron transport in graphene is anisotropic, with the electronic band structure being gapless in the K-point of the Brillouin zone. This unique property enables GFETs to operate in a highly efficient manner, offering superior performance compared to conventional silicon-based transistors.

2. Fabrication of GFETs

The fabrication of GFETs involves several steps, including the deposition of graphene onto a substrate, the definition of the channel region, and the formation of gate electrodes. The most common methods for depositing graphene include chemical vapor deposition (CVD), epitaxial growth, and exfoliation. Once the graphene layer is deposited, it is patterned using photolithography or etching techniques to define the channel and gate regions. The gate electrodes are typically formed using metals such as tungsten or molybdenum, which are deposited by physical vapor deposition (PVD) or chemical vapor deposition (CVD) techniques.

3. Applications of GFETs

GFETs offer several advantages over traditional silicon-based transistors, making them ideal for a wide range of applications. These include high-speed operation, low power consumption, and compatibility with printed electronics. GFETs are particularly useful in emerging technologies such as flexible electronics, stretchable sensors, and wearable devices. Additionally, GFETs can be integrated into nanowire transistors, which can further enhance their performance and scalability.

4. Conclusion

In conclusion, GFETs are a promising technology that showcases the potential of graphene as a material for next-generation electronic devices. With ongoing research and development, GFETs are expected to play a significant role in the advancement of nanoelectronics and related fields. Future work in this area will focus on improving device performance, reducing defect density, and exploring new applications.

Fig. 1 Single layer graphene that is known as a mass detector.

- Graphene Field Effect Transistors (GFET)


A nanoparticle with 30 Fe atoms on the top of defect No. 3

Fig. 2 An iron nano cluster on the top of a defected single layer graphene

Table 1 Interfacial parameters of equivalent Lenard-Jones potential

<table>
<thead>
<tr>
<th>Interaction</th>
<th>$\sigma$ (Å)</th>
<th>$\epsilon$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe-Fe [11]</td>
<td>3.41</td>
<td>0.00239</td>
</tr>
<tr>
<td>C-C [11]</td>
<td>3.41</td>
<td>0.00239</td>
</tr>
</tbody>
</table>

1. Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)
2. Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO)
3. Embedded atom method (EAM)

Eij = 4εσ(σ/\(r_{ij}\))^{12} − 2εσ(σ/\(r_{ij}\))^{6}

$\sigma_{C-Fe} = \frac{\sigma_{C-C} + \sigma_{Fe-Fe}}{2}$

$\epsilon_{C-Fe} = \sqrt{\epsilon_{C-C} \times \epsilon_{Fe-Fe}}$

From the [11] paper, we use 30 Fe atoms on the top of the defect of a single-layer graphene.

$$E_{ij} = 4\varepsilon\left(\frac{\sigma}{r_{ij}}\right)^{12} - 2\varepsilon\left(\frac{\sigma}{r_{ij}}\right)^{6}$$

$$\sigma_{C-Fe} = \frac{\sigma_{C-C} + \sigma_{Fe-Fe}}{2}$$

$$\epsilon_{C-Fe} = \sqrt{\epsilon_{C-C} \times \epsilon_{Fe-Fe}}$$

Table 1 shows the interfacial parameters of equivalent Lenard-Jones potential for Fe-Fe and C-C interactions.

1. Atomic electron density
2. Lenard-Jones potential (LJ)
3. Lorentz-Berthelot (L-B) mixing rule
4. Velocity-Verlet integrator

A nanoparticle with 30 Fe atoms on the top of defect No. 3.
شکل 3: بخش 1 ناحیه سرد و بخش 20 ناحیه گرم در نظر گرفته شده است. پس از اعمال حرارتی لازم برای ناحیه گرم، و گرفتن همان شرایط گرم شده ناحیه سرد، برای دمای در نواحی میکرو (کتا 19) محاسبه می‌شود.

شده تنها تحت هنگرگ کانوی متعادل شود پس از نیروی نور آزمایشی تابش نیروی شیمیاسازی

200ns

2- محاسبات حرارتی حرارتی

در حالات مکانیکی، طبق قانون فوریه از رابطه (6) محاسبه می‌شود.

\[ k = \frac{I}{2\pi A \cdot \Delta T} \]

3- ناحیه میکرو نانوتور و اثر طول‌های مختلف در آن ناحیه می‌دهد.

مقدار طول‌های حرارتی برای طول 12 نانومتر به روش 83nm گیاه 92.3 W/mK کارش داده است. همچنین برای طول 12 نانومتر در [15] برای طول 121 W/mK کارش داده است. منحنی برای طول‌های مختلف نانوتور گیاه آزمایشی است. شکل 5 محاسبه بین ناحیه کارش و مراجعه مدارش با رابطه طول‌های حرارتی برحس طول‌های مختلف نانوتور را نشان می‌دهد. همان‌گونه که ملاحظه می‌شود، طبق رسان‌گذاری بین نتایج دیده می‌شود شکل 6 محاسبه.

4- یکی از روش‌های محاسبه می‌تواند برای اطمینان از بخش از حرارتی برای نانوتور گیاه زیرکاکت باعث برای آزمایش در [9] و [16] می‌شود. همچنین در مرحله بعد‌هایی روی نانوتور گیاه معلق در مناطق

۱- Nose-hoover thermostat

منبع: مجله ماده فیزیکی، سال 1995، شماره 16، صفحه 1

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Effect of length of nano ribbon on the temperature gradient of suspended graphene

Fig. 4

Comparison of thermal conductivity of non-defected zigzag graphene nano ribbon

Fig. 5

Effect of defect location on the temperature gradient of suspended graphene nano ribbon

Fig. 6

Effect of defect location on the thermal conductivity of suspended graphene nano ribbon

Fig. 7

1- Mean Free Pass (MFP)

شکل 7: نمودار اثر مکان عبور بر ضریب هدایت حرارتی نانوتونر گرافن مطلق

سامانه‌های گرافنی به‌طور کلی استفاده شدند.

شیب‌های ارائه نانوتونر فلزی بر همبستگی

شکل 4: نمودار اثر طول کارگاه‌های حرارتی نانوتونر گرافن مطلق

شکل 5: مقایسه ضریب حرارتی حرارتی نانوتونر گرافن زیگ‌زا بدون عبور

شکل 6: نمودار اثر مکان عبور بر گرادیان حرارتی نانوتونر گرافن مطلق

منبع: همایش بین‌المللی مدیریت فروش 1395، دوره 16، شماره 1.
Fig. 8 Effect of metallic nano particle concentration on the thermal conductivity of suspended graphene nano ribbon

Fig. 9 Thermal conductivity of suspended graphene nano ribbon when there are metallic nanoparticle and also when defects are placed with them

Fig. 10 Thermal conductivity with respect to the various diameters of defects on the middle of suspended graphene nano ribbon (alone defect and simultaneous nanoparticles and defects)

1- Relaxation time
2- Phonon Density of States (DOS)
Fig. 11 Comparison of heat path directions (passage channel) of two thermal lines on the top and bottom of middle line of graphene sheet for defects with diameters as size as 2.1 and 3.6 nm and 5 nm wide

- **Heat Sink**
- **Heat Source**

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**Fig. 11**: Comparison of heat path directions (passage channel) of two thermal lines on the top and bottom of middle line of graphene sheet for defects with diameters as size as 2.1 and 3.6 nm and 5 nm wide.

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**References**


[35] M. Boyikata, E. Borges, J. Braga, J. Belchior, Size evolution of structures...