Surface electric field and adsorption properties of noble metal modified graphene in methane gas

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Abstract. Based on COMSOL Multiphysics software, the geometric model of graphene structure is set on the two-dimensional plane, and the thickness of graphene layer is set at 400 nm. The real and imaginary parts of the refractive index of graphene are defined. Then, the Ag and Au films are coated on both sides of graphene to form the Ag/G/Ag and Au/G/Au sandwich structures, respectively. In addition, the electric field modes between 300 nm and 600 nm are obtained by parameterized scanning calculation of the incident wavelength $\lambda$. At the same time, adsorption, scattering and extinction spectra are plotted. Results indicated that the maximum field strength of both the Ag/G/Ag and Au/G/Au sandwich structures are nearly doubled as compared to the intrinsic graphene. Finally, the adsorption, scattering and extinction properties are discussed. It is concluded that the resonance absorption peaks can be adjusted and improved by Ag/Au modification. The strongest plasma resonance mode shifts towards high energy. Moreover, Ag/G/Ag has stronger surface plasmon resonance effect than that of Au/G/Au structure.

1. Introduction

Graphene has been widely investigated due to its unique photoelectric properties. Such as, the structural, electrical evolution and optical properties of graphene induced by oxygen-related defects are investigated [1]. Lounis et al. [2] investigated the interaction between epitaxially grown graphene and SiC substrate using photoluminescence spectroscopy. Wu et al. [3] develop a high-efficiency technology to produce graphene paper with ultra-high thermal conductivity and large quantities. We also discussed the optical properties of graphene [4].

In addition, noble metal have strong local surface plasmon resonance (LSPR) characteristics related to the composition, morphology and size. Chen et al. [5] reported the LSPR of gold (Au) nanoparticles with different shapes and sizes, and investigated the response of their surface plasmon peaks to the refractive index of the surrounding medium. Ugwuoke et al. [6] presented a simplified model of plasmon hybridization and investigated the weak coupling regimes of solid and cavity plasmons in the core-shell nanostructures. Simone and Ruijter [7] demonstrated the surface plasmon resonance and surface-enhanced Raman scattering on a flat Au surface. In addition, plasmonic properties of Al-Ag alloys nanoparticles have been studied [8].

However, the application of graphene is limited due to intrinsic graphene is a gapless semiconductor. In this situation, previous literatures reported that noble metal modification can be used to improve the photoelectric properties of graphene. Lee et al. [9] assembled Au nanocrystals onto graphene and found that the surface enhanced Raman scattering depend on the morphologies of
Au nanocrystals. Zhao and Wu [10] concluded that noble metal (Rh, Pt, Pd) decorated graphene have higher adsorption ability, higher charge transfer and higher orbital hybridization than that of intrinsic graphene. Sharma and Rabinal [11] prepared graphene-silver nanoparticle composites for effective solar absorption by coupling surface plasmon and optical absorption of individual phases. Nair et al. [12] deposited Au on a monolayer graphene and proved that some of the gold are intercalated between the monolayer and the buffer layer.

Interestingly, noble metal modified graphene will produce coupling effect, which will improve the electric field distribution. This widens the resonant bandwidth of the semiconductor and expands the working range of noble metal LSPR. These provide the possibility to improve the detection sensitivity. Therefore, the noble metal modified graphene can be used as a candidate material for LSPR sensor with applications in environmental monitoring. For this reason, understanding of the plasma effect in noble metal modified graphene is of fundamental importance as well as of practical interest for application in sensor devices. Especially, silver is favored by researchers due to its small dielectric constant and suitable price. In this paper, a two-dimensional graphene plane model is established by COMSOL Multiphysics software, which replaces the thin layer structure of graphene. Then, the Ag and Au films are coated on both sides of graphene to form the Ag/G/Ag and Au/G/Au sandwich structures, respectively. The surface electric field of sandwich structures in methane gas are calculated, and their absorption, scattering and extinction spectra between 300 nm and 600 nm are plotted.

2. Model and method

Based on COMSOL Multiphysics software, the geometric model of graphene structure is set on the two dimensional plane, and the thickness of graphene layer is set at 400 nm. The refractive index of graphene is obtained from reference [13].

\[ n_g = 3 + \frac{1}{3} \frac{C_1}{\lambda} \]  

(1)

Where, \( \lambda = 400 \) nm is the wavelength of incident light, \( C_1 = 5.446 \) μm\(^{-1}\), the real and imaginary parts of the refractive index of graphene are 3 and 0.72613, respectively. Then, the Ag and Au films are coated on both sides of graphene to form the Ag/G/Ag and Au/G/Au sandwich structures, respectively. Finally, the electric field modes between 300 nm and 600 nm are obtained by parameterized scanning calculation of the incident wavelength \( \lambda \). At the same time, adsorption, scattering and extinction spectra are plotted.

3. Results and discussion

Figure 1 displays the schematic diagram of Ag/G/Ag and Au/G/Au sandwich structure. The thickness of graphene layer is set at 400 nm. The Ag and Au films are coated on both sides of graphene to form the Ag/G/Ag and Au/G/Au sandwich structures, respectively. The wavelength of incident light is \( \lambda = 400 \) nm.

Figure 1. Schematic diagram of Ag/G/Ag and Au/G/Au sandwich structure.

Figure 2 shows surface electric field of noble metal modified graphene in methane gas: (a) intrinsic graphene, (b) Ag/G/Ag and (c) Au/G/Au. The Ag and Au films are coated on both sides of graphene to form the Ag/G/Ag and Au/G/Au sandwich structures, respectively. At \( \lambda = 460 \) nm, the electric field enhancement can be observed on the right side of the intrinsic graphene. Compared with the intrinsic graphene, there is almost no electric field on both sides of graphene after modifying by Ag and Au films, while their maximum field strength is nearly doubled. This indicates that the sandwich structures have stronger absorption and scattering. In addition, the noble metal modification makes the
surface and the nearby area of graphene have a strong near field enhancement. These provide the possibility to improve the detection sensitivity. Therefore, the noble metal modification graphene can be used as a candidate material for LSPR sensor with applications in environmental monitoring.

**Figure 2.** Surface electric field of noble metal modified graphene in methane gas: (a) intrinsic graphene, (b) Ag/G/Ag and (c) Au/G/Au.

Figure 3 presents adsorption spectra of noble metal modified graphene in methane gas: (a) intrinsic graphene, (b) Ag/G/Ag and (c) Au/G/Au. For intrinsic graphene, four adsorption peaks at 2.43 eV, 2.54 eV, 2.64 eV and 2.89 eV are observed. The intensity of the absorption peak attains the maximum at 2.64 eV. As Ag films are coated on both sides of graphene to form the Ag/G/Ag sandwich structures, all the adsorption peaks related to intrinsic graphene disappear, and the strongest absorption peak shifts towards high energy (3.11 eV). The results show that the position of resonance absorption peaks can be adjusted by Ag modification. However, there are four strong resonance absorption peaks in Au/G/Au structure, indicating that the surface plasmon resonance absorption is enhanced by Au modification.

**Figure 3.** Adsorption spectra of noble metal modified graphene in methane gas: (a) intrinsic graphene, (b) Ag/G/Ag and (c) Au/G/Au.

Figure 4 displays extinction spectra of noble metal modified graphene in methane gas: (a) intrinsic graphene, (b) Ag/G/Ag and (c) Au/G/Au. The change of extinction peak is very sensitive to the modification of noble metal. The noble metals modification can obviously enhance the surface plasmon resonance of sandwich structures, which makes the extinction peak of Ag/G/Ag and Au/G/Au
become stronger, and the strongest plasma resonance mode shifts towards high energy. Moreover, Ag/G/Ag has stronger surface plasmon resonance effect than that of Au/G/Au structure.

**Figure 4.** Extinction spectra of noble metal modified graphene in methane gas: (a) intrinsic graphene, (b) Ag/G/Ag and (c) Au/G/Au.

Finally, scattering spectra of noble metal modified graphene in methane gas are discussed, as shown in Figure 5. Compared with the absorption and extinction properties, the absorption of Au/G/Au is greater than that of scattering efficiency. On the contrary, Ag/G/Ag has higher scattering efficiency.

**Figure 5.** Scattering spectra of noble metal modified graphene in methane gas: (a) intrinsic graphene, (b) Ag/G/Ag and (c) Au/G/Au.

4. Conclusions
The surface electric field of intrinsic graphene, Ag/G/Ag and Au/G/Au sandwich structures are calculated by COMSOL Multiphysics software. Results indicated that the maximum field strength of both the Ag/G/Ag and Au/G/Au sandwich structures are nearly doubled as compared to the intrinsic graphene. In addition, adsorption, scattering and extinction spectra are discussed. It is concluded that the absorption peak intensity of intrinsic graphene attains the maximum at 2.64 eV. As Ag films are coated on both sides of graphene to form the Ag/G/Ag sandwich structures, all the adsorption peaks related to intrinsic graphene disappear, and the strongest absorption peak shifts towards high energy (3.11 eV). The results show that the position of resonance absorption peaks can be adjusted by Ag modification. However, there are four strong resonance absorption peaks in Au/G/Au structure,
indicating that the surface plasmon resonance absorption is enhanced by Au modification. Moreover, Ag/G/Ag has stronger surface plasmon resonance effect than Au/G/Au structure. These results have theoretical and practical significance for the design of noble metal modified graphene optical sensors.

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