SUMMARY OF DOCTORAL THESIS

The author's name: Do Chi Nghia

Thesis title: *Theoretical models and simulations of plasmonic nanostructures for photothermal and biosensing applications*

Scientific branch of the thesis: Physics

Major: Theoretical and Mathematical Physics **Code:** 9 44 01 03

The name of postgraduate training institution: Hanoi Pedagogical University 2

1. Thesis purpose and objectives

1.1. Thesis purpose

The research purpose of the thesis is to develop current Mie theory to study the plasmonic properties of nanostructures investigated in experiments and simulations. Study of temperature variation of these plasmonic nanostructures under laser illumination, to discover new properties and structures to optimize the efficiency, and to exploit how to use the photothermal effect of the system in various applications.

1.2. Thesis objectives

Theoretical study of plasmonic properties of nanostructures including core-shell nanoparticles such as nanoflowers, composite nanostructures based on graphene: graphene on bulk substrate, graphene-coated SiO_2 nanoparticles and a square lattice of graphene nanodisks on a diamond-like carbon thin film grown on a silicon substrate. Investigating the photothermal effect of these plasmonic nanostructures under laser illumination and propose how to use the photothermal effect of these systems in various applications.

2. Research methods

The thesis uses semi-empirical modeling method to study the plasmonic properties of the nanostructures. Specifically, the Mie theory and its improvements are used to determine optical spectra of core-shell nanosystems, especially for nanoparticles and graphene-coated nanoparticles. For composite nanostructure composed of a square lattice of graphene nanodisks on a diamond-like carbon thin film grown on a silicon substrate, we apply quasistatic approximation combined with dipole approximation to determine the polarizability of a single graphene resonator from which the absorption and extinction cross sections can be calculated. Along with that, complicated analytical calculations for photothermal effect have been given that continuum mechanics theory and solving heat transfer and diffusion equations, combining numerical methods, simulation methods and data analysis using Fortran and Matlab software. Compare the results obtained with the experimental data and research results of other authors.

3. Major results and conclusions

3.1. The major results

- Developing the Mie theory studying plasmonic properties (absorption, scattering and extinction spectra) for core-shell nanoparticles. This complete Mie theory can be accurately calculated to a system of 160 nm size when it is compared to experimental data.
- Exploring the optical properties and the thermal-induced stress in the surroundings of heated Ag@Fe_3O_4 nanoflowers in different media using the Mie theory and continuum mechanics theory. Using laser irradiation leads to temperature rise that generates the strain field inside nanoflowers and their ambient surrounding environment. The thermal stress variation has been analytically found. The long-range stress decays as the inverse of the distance and this finding is in a good agreement with previous study. The stress components in silica decay almost as the inverse cube of the distance near the outer surface. As a result, laser-induced thermoelastic effects can be exploited to detect defects in substances and devices.
- Theoretically study the plasmonic properties of graphene on bulk substrates and graphene-coated nanoparticles. The surface plasmons of such systems are strongly dependent on bandgap and Fermi level of graphene that can be tunable by applying external fields or doping. An increase of bandgap prohibits the surface plasmon resonance for GHz and THz frequency regime. While increasing the Fermi level enhances the absorption of the graphene-based nanostructures in these regions of wifi-waves. Some mechanisms for electric-wifi-signal energy conversion devices are proposed. Our results have a good agreement with experimental studies and can pave the way for designing state-of-the-art electric graphene-integrated nanodevices that operate in GHz-THz radiation.

- Investigating the plasmonic heating of graphene-based systems under irradiation of a mid-infrared laser. The nanostructures comprise a square array of multilayer graphene nanodisks deposited on the diamond-like carbon thin film, which is supported by a silicon substrate. While illuminating the systems by the laser light, plasmonic nanodisks absorb more optical energy than the counterparts without graphene and convert to thermal dissipation. This finding indicates that the ohmic loss is much larger than the dielectric loss in the mid-infrared regime. An increase in graphene plasmonic layers enhances the thermal gradients. At fixed number of graphene layers, the temperature increase is linearly proportional to the optical power and decays as the inverse square of the laser spot. Furthermore, a decrease in the heated temperature, as increasing the thermal conductivity of the thin film layer, is also calculated and discussed.

3.2. Conclusions

- The research results of the thesis are reliable and have been published in ISI journals: *Physica Status Solidi-Rapid Research Letters* (Q1), *Journal of the Physical Society of Japan* (Q2), and in Scopus journal: *Journal of Science: Advanced Materials and Devices* (Q1).
- The thesis proposes the first semi-empirical research direction in Vietnam on the plasmonic properties of nanostructures and its photothermal applications, so that it can be combined with experimental groups to explain the results and propose new applications. This method is quite simple, has been published in prestigious scientific journals and can completely help experimental groups verify data and predict the results of new generation nanostructures.