IOSR Journal of Biotechnology and Biochemistry (IOSR-JBB)
ISSN: 2455-264X, Volume 4, Issue 4 (Jul. – Aug. 2018), PP 83-87
www.iosrjournals.org

Near Field Optical Properties of Aggregated DNA particles

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ABSTRACT
Surface enhanced Raman scattering (SERS) is observed in highly conducting materials such as gold and silver. Near field calculations of light scattering is exetended to bio-molecules and bio-molecules on gold nanometer plate. Near field optics of scattered light from DNA aggregate in spherical shape is theoretically considered. The spherical DNA molecules aggregate is placed on a gold nanoplate to ascertain its near field optics. Two different type materials- irregular shaped dielectric materials on gold nanoplates are considered in near electric field calculations. These surface enhanced scattering are calculated for non-spherical shapes by approximate methods.

I. INTRODUCTION

Recently, new interest for the study of the local electromagnetic fields near nanostructures resulted from recent developments in nanofabrication [Gates et al. (2005), Biswas et al.(2012)] and nanocharacterisation techniques [Pana et al. (2010), Gillet & Meunier (2005)] along with near-field scanning microscope improvements [Betzig & Trautman (1992)]. It is now clear that nanostructure shapes affect the various optical properties, hence the need to study the angle-dependent scattering properties of non-spherical nanoparticles.

The electromagnetic field near to the scattering object and far from it, may have different spatial distribution as well as magnitude. In particular, due to coherence effect and/or plasmon oscillations, the field inside and near the nanoparticles is often enhanced in comparison to the incident field. It was observed that pyridine adsorbed onto the surface of metal (Ag, Cu or Au) nanoparticles, exhibit greatly enhanced Raman scattering intensities ([Jeammarie & Van Duyne (1977), Albrecht & Creighton (1977)]). Theoretical calculation of this enhancement in intensity is computed using exact and approximate methods.

A few very precise numerical techniques are available for such a study. One of the most versatile tools is the Discrete Dipole Approximation (DDA), in which the target is discretized, that is represented by a dense arrangement of identical small dipoles covering the geometry ([Purcell & Pennypacker (1973), Draine (1988)]). The dipoles are placed on the nodes of a regular simple cubic lattice. In principle, the DDSCAT code can be used for any arbitrary shape ([Draine & Flatau (1994)]) and is available for free (Draine's website). In the version DDSCAT 7.3 or later, the electric field intensity near the scattering particles and inside it, can be calculated. This provides a precious tool to study the distribution of the scattered electric field in the nearby space.

Hereafter, we compute, using the DDSCAT code, the electric field distribution near and inside nanoparticles of different shapes of equal volume. We focus on the 'enhancement factor', $Q(=|E_{loc}|^2/|E_{inc}|^2)$, here defined as the ratio between the intensity of the electric field (E_{loc}) at the surface and the intensity of the incident field (E_{inc}). For the small (*i.e.* size parameter << 1) nanoparticles, the enhancement factor is proportional to the squared polarizability, α^2, with $\alpha \propto (\varepsilon_p-1)/(\varepsilon_p+2)$ and ε_p is the dielectric constant of the particle. Close to the Fröhlich frequencies for which the dielectric constant $\varepsilon_p = -2$, optical resonance leads to the maximum possible enhancement of these small nanoparticles (Anderson (2003)). This can be realized essentially for small metallic nanoparticles. Note that in this case, the enhancement factor is proportional to the squared volume of the particles, then this parameter *Q* does not depend on the definite shape of the nanoparticle.

In the present article we investigate on near field optics of nanoparticles or large molecules such as DNA molecules which are non-conducting in nature, possibly deposited on a metallic substrate.

II. METHOD AND CALCULATION

The study mainly consists of two parts- in the first part we consider the non-conducting particle of DNA molecules in spherical shape. Spherical aggregates of DNA molecules (hereafter DNA ball) is studied as an isolated particle and the same aggregated particle is placed on a nanometer sized gold base in second part. Aggregation of DNA sample in ball shape is used in calculations to determine near electric field near and inside the isolated sample. This is particularly a theoretical approach to calculate the field intensities for group of

molecules based on Au-base useful in SERS technique. The electric field intensity near to grain is shape dependent and this is continued to level of single DNA molecule.

DDSCAT technique is already utilised to study optical properties of DNA molecule (Shapiro et al.,1994; Umazano & Bertolotto, 2008). Electrical field calculations in Mie theory or DDSCAT method need refractive Index data. Refractive index of DNA molecules can be determined by using water based solutions of different concentrations of DNA molecule. We have used it from – 'Optical properties of DNA in the extreme Ultraviolet' (T. Inagaki, R. N. Hamm & E. T. Arakawa). Calf thymus DNA was used in their study in determining refractive index.

Theoretical calculations for SERS enhancement have done using Discrete Dipole Approximation (DDA) method or Finite-Difference Time-Domain (FDTD) method apart from Mie theory estimates (Schatz, Young & Van Duyne (2006)). Computations of the SERS enhancements in this paper are done using the DDA method with a precise Clausius-Mossotti relation corrected by lattice dispersion relation and 3rd order radiative term ([Draine & Goodman (1993)]). We have utilized DDSCAT 7.3 to calculate near electric field of scattered light from DNA molecules aggregate.

The particle volume is expected to be statistically same here for all shapes of particles. This choice can be written in term of the same equivalent radius (we have chosen randomly equal to 0.1125 m (or 112.5 nm). In theoretical estimates nanoparticle is further placed on a gold base to determine enhancement after non-conducting particle is placed on conducting base (Figure 1). Similarly, discretization required by DDSCAT code is realized using the same number of dipoles for all the particles and a wavelength is fixed to the value 0.5 μm. Value of the refractive index depends on the material (DNA molecule or gold).

III. RESULT AND DISCUSSION

The spherical particle

One can see that target geometry is represented as dipoles placed on cubic lattice in figure (1). The high-symmetry of the spherical particle exhibits symmetry in the scattered electric field distribution. The wavelength of incident light on aggregate nano-particle of DNA molecules is 0.5 μm.The calculations are done for the wave incident along x-axis. The figure (2) shows the plot of |Eloc|2//|Einc|2inside and around the DNA ball.

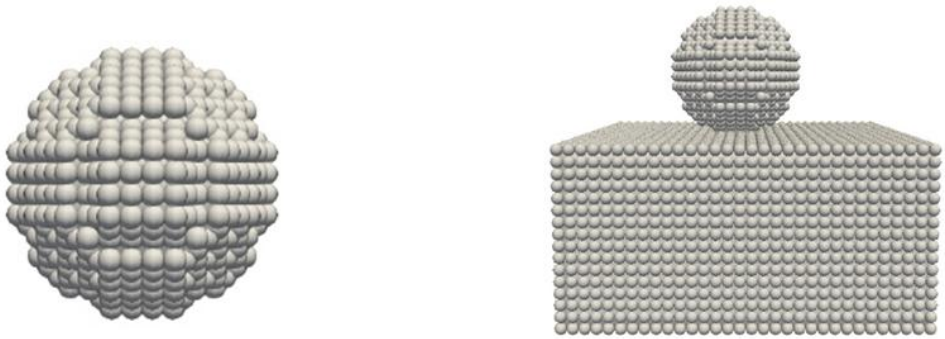

Figure 1: Spherical nano-particle aggregate of of DNA molecule of radius 0.1125 μm and same DNA aggregate placed on gold base. The number of dipoles and dimensions of the DNA ball is same in both cases.

Isolated particle and Particle on Gold base:

For the experimental purposes we need to place the nanoparticle on a suitable base. The calculations are further extended for even smaller nanometer sized particles and a comparative study is made when these particles are place on a very small gold base. Thus a non-conducting organic nano- particle is studied as isolated particle and also placed on gold base. Such a well arranged gold base at nanometer scale is considered theoretically. The study is conducted for the DNA ball having total number of dipoles equal to 912. The gold square base has dimension nearly 0.27 μm and same aggregates of DNA molecules of radius 0.1125 μm is placed on this base. The particle's position on the gold base is shown in the figure (1). The volume of this nano-particles assembly is equal to that used in earlier calculation for isolated spherical DNA molecules aggregate.

The DNA near field optics:

We have investigated the optical properties of isolated DNA aggregation. We see the difference in near field optics of theoretically predicted calculation of isolated DNA ball and when it is placed on probe base. Theoretical calculations are assumed on the basis of imaginary experiment of Raman scattering. It is supposed that a very low concentration of DNA molecule in water solution drop is placed on a gold probe and water is allowed to evaporate and we are left with DNA molecules aggregated as spherical particle on the probe to be

used in theoretical scattering experiment. This gold base rather needle of few nanometer in size if achieved is very sensitive to mechanical and physical condition in the laboratory. It is also supposed that due to surface tension aggregation of molecules on the probe will take place. So we have conducted two type of study for DNA molecules- aggregates placed on gold base and isolated single DNA molecule.

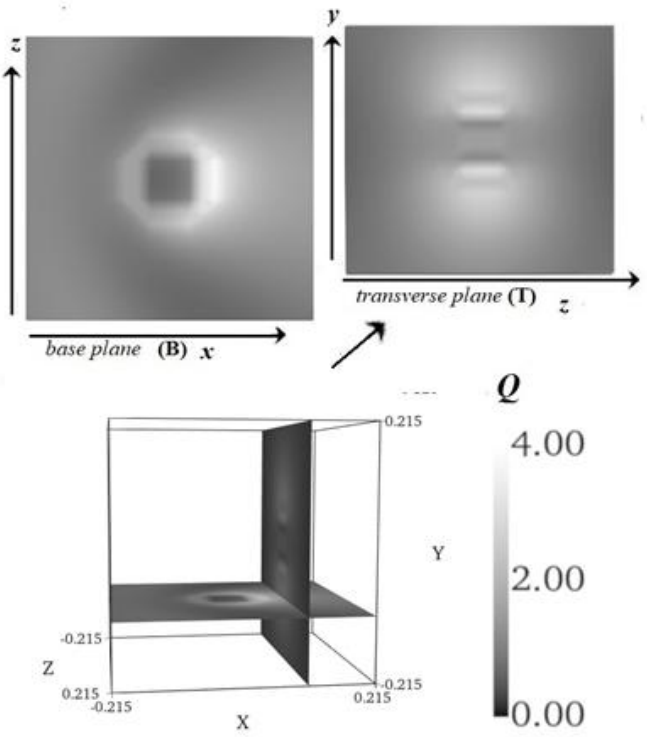

Figure 2: *Intensity of the electric field near and inside the homogeneous particle of radius 0.3 m made of aggregates of DNA molecule. The incident electromagnetic wave of wavelength 0.5 m is of intensity unity and is polarized along the z-direction. It propagates among the x-direction. The spatial scale in the figure is in μm.*

AGGREGATES OF DNA

Spherical DNA Ball

Spherical ball of radius 0.3 μm containing molecules of DNA is shown in Figure 2. The enhancement in electric field is observed near the surface sphere in opposite direction of incident beam. The electric field vector of incident light polarizes electrons in two opposite directions. These electrons are responsible for enhanced surface glowing at two ends. One noticeable point can be observed that instead of a shadow in backward direction we see the glowing surface. The scattered field has clearly two loaves of symmetric field distribution. In particular, the intensity of the electric field pattern for the homogeneous spherical particle has a two-fold symmetry distribution; symmetry along the y-axis when the incident wave has the electric field is along y-axis. The electric field vector polarizes the electron in two opposite directions as earlier in case of sphere. It should be noted here that this plot is for a particular fixed dielectric constant at particular wavelength.

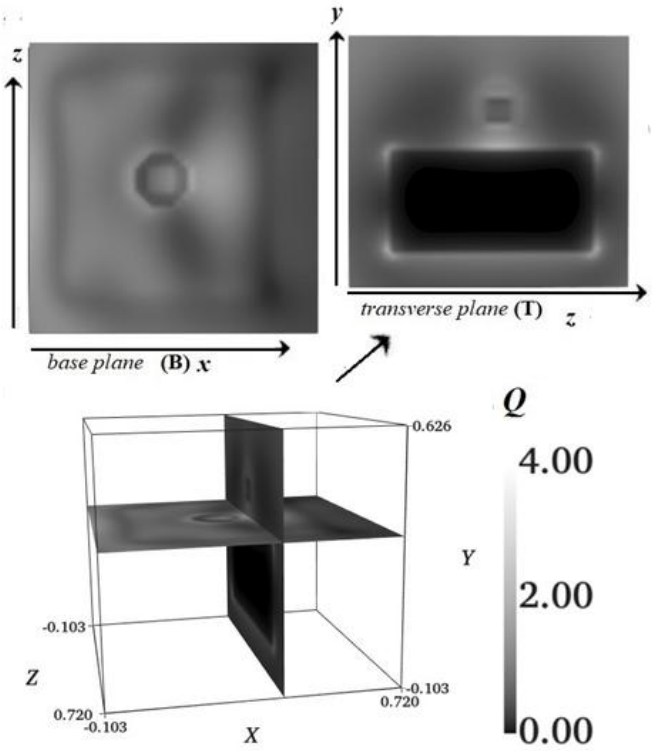

Figure 3: Square of electric field (E) in near Field region is shown and dimensions are in μm. Spherical compact aggregation of DNA molecules placed on a gold probe and results are shown in figure for Wavelength is 500 nm.

DNA BAll on Gold base

The same DNA aggregates smaller in size is now placed on a gold base as in previous paragraphs. The volume of this theoretical nanometer sized DNA aggregates on the gold base is still equal to volume of spherical aggregate of DNA molecules. We considered 17296 number of dipoles out of which 912 dipoles are that of the DNA ball in calculation as shown in figure 1.

The intensity of electric field distribution for the spherical nano-particle of aggregates of DNA molecules on gold base is shown in figure (3). Inside the base the field intensity is poor but the surface is glowing. There is a bit contradictory result is obtained with amorphous carbon placed gold base is that instead of creating a shadow, it creates a radiating shadow of amorphous carbon. The edge of the gold base glitters more than the adjoining surfaces. This can be understood with more electrons at the edge of the base than on the surface. The calculations with non-conducting materials depict same enhancement but intensity may differ. The edge of gold is also shining due concentration of electrons at the edge. Intensity of the scattered light is very poor and is hard to detect the DNA grain, but it clearly marks on the gold base as enhancement. This is clearer from second graph, where E2 is direct measurement of intensity. Shadow on the gold glimpses the shape of the particle.

IV. CONCLUSION

In our calculations involving single particle, shape of the particle has its effect in near field calculations and simply it is not only increase in near field. Different shapes left its print on gold base as glowing or enhanced local field as anti-shadow. We have considered non-conducting material biomolecule DNA in calculations. Thus SERS can be a powerful tool to estimate the shape.

A possible method for DNA detection is developed by Braun et al. (2007) by creating silver hotspots in its double helix. Experimental techniques are being used. Our method theoretically investigate the possibilities of detecting DNA or aggregates by placing it on the gold base. We have conclusions on the basis of the calculations for particle on gold base – The shapes clearly show the differences in pattern observed on the gold bold base. Shapes emerge as a bight shadow opposite to that we see. So gold base serve as an anti-mirror on which a glowing shadow emerges. Thus an estimate of the nanoparticle shape can be made based on these images.

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