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Effect of the probe location on the absorption by an array of gold nano-particles on a dielectric surface

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ABSTRACT

Effect of silicon atomic force microscope probe position and particle spacing on the local absorption of an array of gold nanoparticles placed over a dielectric borosilicate glass surface are evaluated. An improved, vectorized version of discrete dipole approximation coupled with surface interactions is employed throughout the study. It is shown that surface evanescent waves interacting with the system of nanoparticles and atomic force microscope probe result in a near-field coupling between them. This coupling can enhance or reduce the local absorption by the nanoparticles depending on the position of atomic force microscope tip in three-dimensional space and direction of propagation of the surface evanescent wave. The position of the atomic force microscope's tip and spacing that maximize the absorption are identified. This concept can be used for selective heating of nanoparticles placed over a surface that enables precision manufacturing at nanometer scales.

1. Introduction

Noble metal nanoparticles (NPs) such as gold (Au) and silver (Ag) are prime candidates for different nano-scale manufacturing, and diagnostic applications, as their responses vary with changing nanoparticle size and incident wavelength. The oscillation frequency of free electrons on the surface of the nanoparticle alters their optical properties. When incident wave frequency and free electron frequency of the nanoparticle match, localized surface-plasmon resonance (LSPR) occurs as discussed in [1,2]. While metallic nanoparticles usually experience high optical absorption at LSPR wavelength, the presence of a dielectric atomic force microscope (AFM) probe's tip can further augment the LSPR absorption [3]. Therefore, AFM tip can be used as a nanofabrication tool as it enables selectively heating and melting of nanoparticles on a surface [4]. The choice of the nanoparticle and AFM tip material is important in regards to their optical properties. While gallium phosphide (GaP), gold and silicon can be used, GaP has negligible absorption and low heat conversion compared to gold structures as studied in [5]. Moreover, comparison of absorption efficiencies of the nanoparticles under the effect of different AFM tip materials showed that dielectric Si AFM tip could heat the nanoparticles more efficiently than the gold AFM tip. Hence, Si AFM tip can be more suitable for the selective heating of gold nanoparticles on a substrate [1]. Besides nanoparticle heating applications, understanding the effect of Si AFM tip placed in the proximity of nanoparticles can be useful for tip-based imaging, sensing, near-field scanning optical microscopy (NSOM/SNOM) and tip-enhanced Raman spectroscopy (TERS) [6–8]. Due to dispersive properties of Si, AFM tip can be considered as an absorbing or non-absorbing depending on the incident wavelength. The LSPR wavelength for this study is in a range where the imaginary part of the refractive index of Si is negligible, and despite the intensified heating of metallic nanoparticles at their resonance wavelengths, the non-plasmonic AFM tip's absorption will be minimal [9]. Therefore, absorption of the tip can be ignored considering AFM tip's size and shape while the tip alters the heating rate of the nanoparticles at LSPR wavelength due to plasmonic coupling.

Solution of the Maxwell's equations is required to understand the effect of electromagnetic (EM) illumination on any object. Computational electromagnetic methods (CEM) are used for predicting the optical properties through solution of the Maxwell's equations. While CEM can be classified as analytical, semi-analytical and numerical, analysis of the arbitrarily shaped objects' behavior requires the use of semi-analytical or numerical methods. The discrete dipole approximation (DDA) is a semi-analytical CEM that can be used to simulate any arbitrarily shaped, non-homogenous, anisotropic object, by representing it by a number of

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dipoles. The general formulation of DDA was initially developed by Purcell and Pennypacker [10]. Since then, the method became a frequently used approach, with many open source DDA implementations such as DDSCAT, written in FORTRAN, developed by Drain and Flatau [11,12], and ADDA, written in C, developed by Yurkin and Hoekstra [13].

When the object placed on a surface is illuminated by an EM wave, the incident field over the object of interest results from the superposition of the direct illumination, its reflection from the surface, and the scattered field by the nanostructure coming from the surface. An analytical formulation of surface interaction for semi-infinite surfaces can be embedded in the standard DDA interaction matrix to prevent the increase in computational time resulting from representing the surface with dipoles. The implementation of the surface effect in DDA was first introduced by Taubenblatt and Tran [14] to model light scattering from particles placed on a semi-infinite surface. Another implementation, DDSURF, was developed by Schmehl and Nebeker [15,16]. While these two implementations were not open source, DDA with Surface Interaction (DDA-SI) that was developed by Loke and Mengüç [17] was the first open source MATLAB^{TM} toolbox available to researchers. The toolbox was verified for plane wave-particle and surface wave-particle interactions against well-known methods such as finite-element method (FEM) and finite-difference time-domain (FDTD) in [1] and MNPBEM toolbox, which is developed based on boundary element method (BEM), in [18]. While these verification studies show a good match for optical properties of a single AuNP on a surface, validations are also carried out using microwave analog experiments for the far-field scattering of absorbing and non-absorbing particles on a dielectric surface [19]. A vectorized version of DDA-SI (DDA-SI-v) is recently developed by the present authors [20] that showed significant improvement in numerical efficiency. More recently, the surface integration by utilizing fast Fourier transform for improving efficiency has also been implemented in ADDA by Yurkin and Huntemann [21].

Localized heating in the order of nanometer scales has been an interest of researchers for nano-manufacturing. Hawes et al. [4] experimentally demonstrated the feasibility of melting or evaporation of 50 to 100 nm gold nanoparticles on a glass surface in close vicinity to a tapping-mode Si AFM tip by a 15 mW 532 nm wavelength laser. The results showed that melting or evaporation of gold nanoparticles occurs only beyond certain thresholds in the particle-probe interaction time. Furthermore, the average distance between the probe and the surface, and between the tip of the probe and the particle are also found to be important [4]. Huda et al. [3,22,23], used finite-element method (FEM) to investigate heating of silver and gold nanoparticles on different substrates with gold and silicon AFM tip probes, and showed that gold AFM tip has a negative effect on the localized absorption efficiency of the gold nanoparticle due to plasmon response of metal arising from the losses of interband transitions at the LSPR wavelength. Moreover, they outlined that non-plasmonic silicon AFM tip can effectively increase the absorption by gold nanoparticle by means of enhancing near-field interaction [23]. While the effect of AFM tip radius, nanoparticle size, and polarization of incident wave are also investigated, it is observed that the transverse magnetic (TM) illumination is more effective than transverse electric (TE) illumination for heating up nanoparticles by coupling. The evanescent wave from TM wave has both perpendicular and parallel components, whereas the wave from TE illumination has only the parallel component [1,3]. In another study, Loke et al. [24] identified the positive effect of an AFM tip on the normalized dipole field intensity of a 20 nm gold nanoparticle that is placed on a surface. More recently, the present authors carried out an optimization study to identify the ideal relative AFM tip position and limits of enhancement for solid and core-shell gold nanoparticles with dielectric core considering evanescent surface wave heating [20]. It was noted that there are several AFM positions, where significant enhancement can be observed, and further absorption enhancement is achieved using core-shell nanoparticles with a dielectric core for a shifted resonant wavelength with respect to that of a solid nanoparticle.

While the interaction of a single gold nanoparticle placed over a glass surface in the proximity of a silicon AFM tip with an incident TM evanescent wave is investigated in [20], more than one nanoparticle should also be considered for practical applications such as in the experimental study of Hawes et al. [4]. The current study is a continuation of [20], where the absorption efficiency limits for a single particle with different AFM tip locations were studied. The effects of neighboring nanoparticles on AFM probe controlled localized heating are investigated by extending the study further, considering an array of nanoparticles and identifying the absorption profile of the particle of interest depending on the spacing of neighboring particles and position of the AFM probe. Therefore, the effect of nanoparticle spacing is compared as a first step to determine the minimum spacing of the array configurations. Moreover, the effect of a high-permittivity silicon AFM tip's position in 3D space relative to different 2D array configurations of gold nanoparticles is investigated to identify an optimal position of AFM tip for maximizing the heating effect on the AuNP in the center. While only the absorption patterns are of concern for this study, the absorption values can be converted to localized heating rates either using macro-scale radiation transfer calculations as presented by [25,26], or by adopting near-field calculations similar to those reported by Francoeur and Mengüç [27], Didari and Mengüç [28–30], Edalatpour et al. [31].

2. Problem statement

The system consists of 9 identical gold nanoparticles with 50 nm in diameter placed on a BK7 borosilicate glass substrate with an AFM probe tip in their vicinity as shown in Fig. 1. The glass substrate is thick enough so that it can be considered as a semi-infinite surface with respect to the length scales considered in this study. In this problem, localized absorption of the center nanoparticle of a 2D array is considered. A monochromatic TM wave is incident from below the surface with an incident angle of 45°, which is greater than the critical angle for the wavelength range of 300 nm and 800 nm. A decaying evanescent wave propagates on the front surface with both vertical and parallel components as shown in Fig. 1, and it interacts with the nanoparticles and the

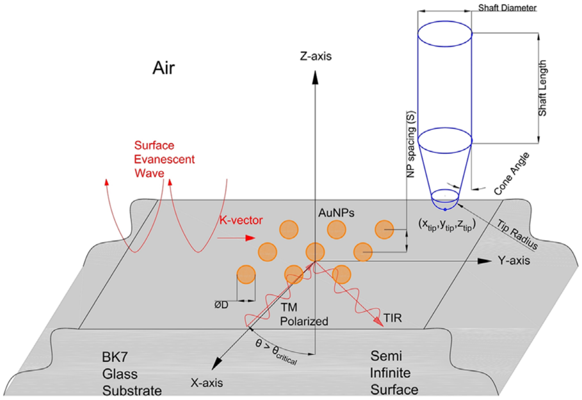

Fig. 1. A schematic view of the configuration. TM wave is incident at an angle larger than that required for TIR from underneath the BK7 glass substrate and the decaying evanescent wave has both *y* and *z* components.