Interaction of nanoparticles on a substrate with an AFM probe: DDA-SI formulation

V. L. Y. Loke[*] and M. P. Mengüç

School of Engineering, Özyeğin University, Kuşbakışı Cad. No:2, Altunizade 34662, Istanbul, Turkey.

Motivated by the need for a modeling tool for nanostructures interacting with a substrate and an AFM probe, we developed a MATLAB implementation of the discrete dipole approximation with surface interactions (DDA-SI). The method is applied to investigate the near-field coupling between particles on the surface and an AFM probe. The results presented here explore the effects of a number of physical, geometrical and material properties that can eventually assist nanolithography, particularly in defining the parameters for nano-writing.

INTRODUCTION

Atomic force microscopes (AFMs) are used to image surfaces with nanometric structures. They can also be used as nanolithographic tools, i.e., to write on a surface by means of melting nanoparticles or the substrate itself [1]. Following from our initial work with free-space-dependent scattering formulations presented for two-particle [2,3] and particle-probe [4] systems, we study the field intensity profiles resulting from near-field coupling of a system comprising an AFM probe, a particle and a surface (Fig 1).

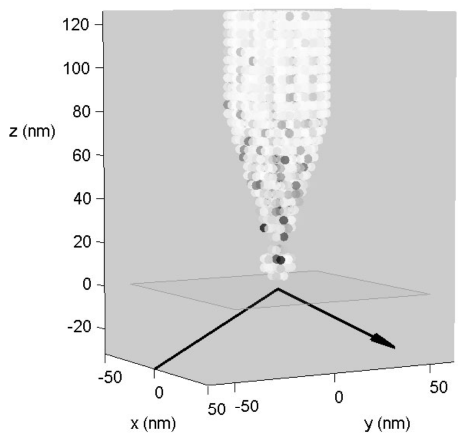

Figure 1. Dipole model of an AFM probe and a particle on a surface. The incident TM plane wave from below the surface is internally reflected; an evanescent wave exists above the surface. The darkness of each dipole is plotted proportionally to the field intensity.

* Corresponding author: Vincent L. Y. Loke (Vincent.Loke@ozyegin.edu.tr)

Our model is based on the discrete dipole approximation (DDA) [5, 6] and its subsequent development that account for surface interactions (Fig. 2). The model does not account for the effect of radiative emission but it is part of the scope of our ongoing development to account for all relevant phenomena in AFM nano-engineering.

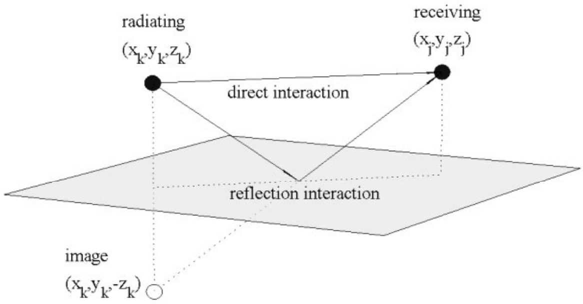

Figure 2. Direct and reflected dipole interactions.

MODELING METHODOLOGY

DDA is widely used to model light scattering from arbitrarily shaped mesoscopic and nanoscale objects in free space. DDA has also been extended to include surface effects of a homogeneous substrate (as per DDSURF [7]) and later for filmed surfaces (DDFILM [8]); our MATLAB implementation is called DDA-SI. The surface interaction involves decomposing spherical waves into cylindrical and planar components [9] which expand in parallel and perpendicular to the surface respectively (Fig. 3); the latter is multiplied by Fresnel reflection coefficients, accounting for the fraction of light reflecting of the plane surface.

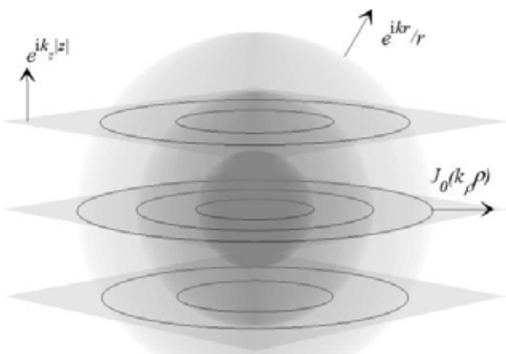

Figure 3. The spherical wave decomposed into cylindrical and planar components.

The system of equations, whose derivation is explained in [7,9], is

$$\sum_{k=1}^{N}\left(\mathbf{B}_j + k_0^2\mathbf{G}_{jk} + \mathbf{S}_{jk} + \frac{k_1^2 - k_2^2}{k_1^2 + k_2^2}k_0^2\mathbf{G}_{I,jk},\right)\mathbf{P}_k = \mathbf{E}_{inc,j}, \tag{1}$$

where the terms $\mathbf{B}_j + k_0^2\mathbf{G}_{jk}$ are equivalent to the free-space interaction matrix $\mathbf{A}_{jk}$ defined in [6] and the other terms account for surface reflection interaction [7]; $\mathbf{B}_j$ is the reciprocal of the dipole polarizability [6], $\mathbf{G}_{jk}$ is the dyadic Green's function of the electric field from a radiating dipole, $\mathbf{S}_{jk}$ contains the essential integrals which comprise Bessel or Hankel functions, evaluated using contour integrals [9] and $\mathbf{G}_{I,jk}$ is the image dyadic Green's function of the field from an image dipole [7]. The linear equations are solved using the generalized minimal residual method (*gmres* function in MATLAB).

RESULTS AND DISCUSSION

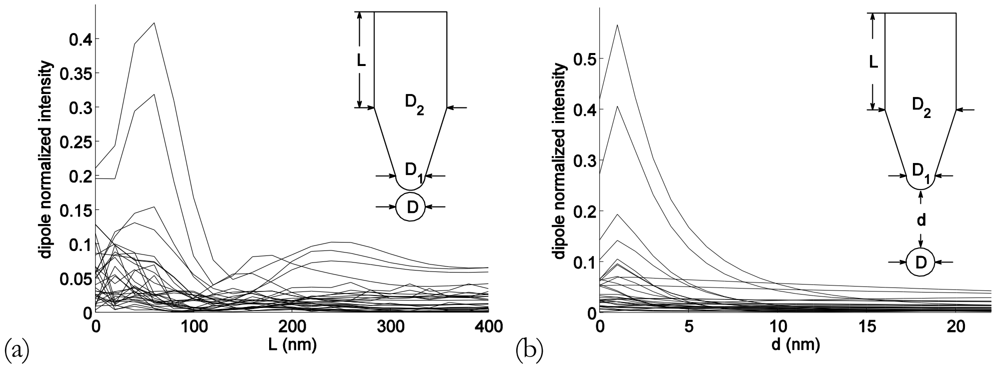

Figure 4. Field intensity of the 32 dipoles that make up a sphere on the surface as a function of the AFM probe a) shaft length, L (const. d=2 nm) b) vertical separation, d, between the tip and sphere (const. L=60 nm). In both cases, D=20, D_1=20 and D_2=50 nm.

The MATLAB implementation of the Sommerfeld Identities was tested against that of [9] which was written in FORTRAN, and the DDA-SI implementation was benchmarked against [10]. Satisfied with the results, we modeled the AFM probe configuration in Fig. 1, illuminated with either TE or TM polarized evanescent waves above the surface. The TE wave has just a component in the x-direction; whereas, the TM wave has both y and z components. As expected, the coupling is stronger in the latter case, which has contributions from the vertical component of the incident evanescent field. The results of the dipole field intensities are shown in Fig 4 and Fig. 5.

Fig. 4a shows the effect of the shaft length on the field intensity; as the shaft gets longer, the reflective effects from the flat top of the truncated shaft, peaking at around L=60 nm, diminishes. However, the effect of the truncated shaft can be exploited to increase near-field coupling. Varying the separation between the AFM probe tip and the particle, we see that the field intensity peaks at d = 1 nm (Fig. 4b). Fig. 5 shows that, for a particular AFM probe-tip separation, there is a corresponding resonance frequency. We continue to investigate the coupling dependence on other parameters and with multi-particle configurations. Although other physical phenomena such as radiative transfer, emission and perhaps Casimir and optical forces need to be considered in order to attain a complete model, the field intensity in the material is a major factor for determining the parameters for melting a particle onto a substrate, e.g., in the nano-writing process.

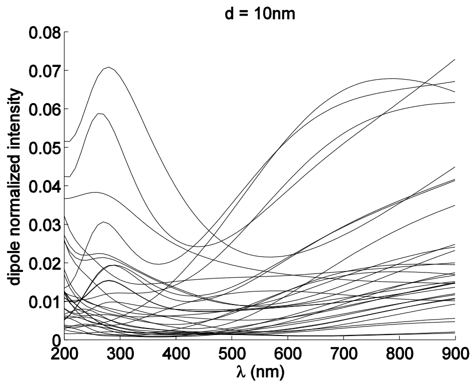

Figure 5. Resonance effect of the AFM probe at a given tip and particle separation.

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