The Effect of Nanoparticle Clustering on Optoelectronic Property

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Abstract

Metal nanoparticles have been extensively investigated for the applications in micro-nano electronics, plasmonics, and chip packaging due to their enhanced thermal, mechanical and electrical properties at the nanoscale. For instance, surface-to-volume ratio and particle distribution significantly affect the sintering and melting behavior of nanoparticles relative to bulk properties. Hence, understanding the characteristic behavior of these materials is vital for the use of these nanoparticles in existing and new applications. It has been shown that at the nanoscale van der Waals forces are the dominant force between particles, which results in particle agglomeration and creates particle clustering. In this paper, we show how this nanoparticle clustering effects the optoelectronic property of the domain by applying the finite difference frequency domain method. This is the first step towards understanding the modeling of the heat transfer that characterizes the laser particle interaction for additive manufacturing using nanoparticles.

Keywords: Nanotechnology, Surface Plasmon Polaritons, Near-Field Energy Enhancement

1. Introduction

The industrial demand for smaller devices have resulted in the development of nanomanufacturing. There has been suggested some methods such as lithography; however, most of these methods are restricted by the diffraction limit of the light and their inability of large area manufacturing. Hence, the development of new methods for metals and ceramics are vital to fabricate additively-manufactured parts with sub-micron scale resolutions which makes the harnessing the heat transfer at the nanoscale become crucial to overcoming the diffraction limit by the creation of near-field heat transfer around the structures [1,2]. There has been some techniques based on near-field optics have been applied to confining the light at the nanoscale. Nanomaterials such as metal nanoparticles have attracted interest as their optical, thermal, and electromechanical properties of nanomaterials are quite different from the properties of the bulk material, and they can be tuned easily by controlling the shape and size of the nanostructure. The noble metals have high electron mobility and are considered good electrical conductors, making them attractive candidates for plasmonic applications. They support the localized surface plasmons (LSPs) and surface plasmon polaritons (SPPs) due to their ability to

enhance the electromagnetic fields and light confinement between metal and dielectric materials. The interaction or coupling of the plasmons on the nanoparticles provide practical strategies to the design of nanostructures. Also, the surrounding dielectric medium changes the plasmonic properties of the nanoparticles which has been big interest in the development of plasmon resonants [3,4]. The resonances have resulted in some exciting applications such as Surface Enhanced Raman Scattering (SERS) and nanoscale sensing, which is manifested by the enhanced scattering and absorption cross sections of nanoparticles. However, understanding of plasmonic nanoparticle clusters is a significant challenge. Recently, metal nanoaparticles have been used in the additive manufacturing of electronics, aerospace and medical device parts through microscale selective laser sintering (μ-SLS) where nanoparticles replace the traditional powders used in standard SLS processes [5, 6]. Hence, many efforts have been devoted to the fabrication of metallic nanostructures by different methods [7]. Different shapes and sizes have been synthesized and plasmonic properties have been studies previously [8]. The plasmonic resonance behavior of some anisotropic nanostructures show different behavior than the spherical metal nanoparticles. For example, the plasmonic resonance peaks of anisotropic nanostructures move towards longer wavelengths, and some anisotropically etched nanoparticles show broad bandwidths [9].

The cohesive interactions between the nanoparticles, dominate interactions between the nanoparticle at nanoscale can result in agglomeration [10, 11]. These agglomeration effects can significantly reduce the packing density of the nanoparticles and show different field enhancement and plasmonic effects compared to the individual metallic nanoparticles. Hence, optoelectronic properties of such agglomeration effects on plasmonic behavior need to be understood well so to be tuned accurately by changing the gap distances and the size of the adjacent nanoparticles [12]. In this paper, we investigate the plasmonic properties of spherical copper nanoparticles with agglomeration effect using finite different frequency domain method. We displayed the near-field intensity enhancement and the movement of the LSPR peaks of the Cu nanoparticles.

2. Modeling Approach

Finite element method shows higher accuracy for modeling the irregular shapes compared to other methods and enables to simulate finite elements within large domain. Khoury et al. have revealed the validity and the accuracy for plasmonic-nanostructure modeling by finite element model [13]. In this study, finite difference frequency domain based on finite element method (FEM) has been used to understand near-field intensity distribution of metallic nanostructures by solving Maxwell's equations. Moreover, the Cu nanoparticles were surrounded with air which the refractive index is taken as n=1 and complex permittivity

of the metallic nanoparticle is used from experimental data from [14]. Also, non-uniform meshes are implemented effectively and produce convergence as well as saving computational time [15].

As the nanoparticles exhibit different plasmonic effects at different size and gap distances, configuration of the particles need to be understood well to be able to tune the optical properties of plasmonics. As the metallic nanoparticles agglomerate at the nanoscale, we used two different configurations in which there are three particles initially are agglomerated in both cases. In the first case, we used linear configuration and in the second case, we analyzed the triangular configuration. The configurations are illustrated in Fig. 1.

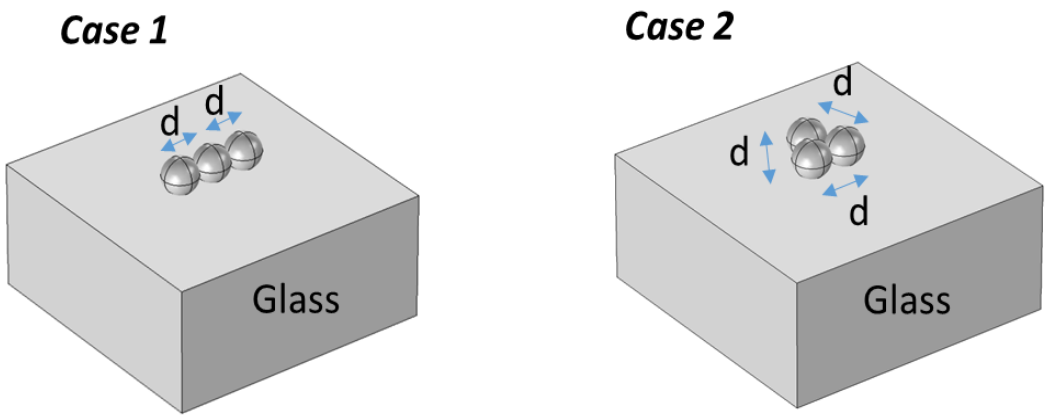

Figure 1. Linear (Case 1) and Triangular (Case 2) Configurations

In this paper, we have analyzed two cases in which the nanoparticles are placed in linear and triangular configurations. We have used copper nanoparticles with 100 nm diameter on a 350 nm thick, 750 nm x 750 nm wide glass substrate.To be able see the agglomeration effect, we have varied the distance between the particles (*d*) from 0 to 50 nm. By investigating TE polarized light, scattering and absorption cross sections are calculated. Scattering cross section is found by calculating the surface integration of the scattered Poynting vector and the absoprtion crosssection is analyzed by the volume integration of the absorbed energy within the nanoparticles. 532 nm wavelength, TE polarized light is irradiated for each cases.

3. Results and Discussion

Fig. 2 shows the linear (Case 1) configuration electric field enhancement for d=0 at the center of the nanoparticles. It indicates that surface plasmons are generated along the polarization direction of the nanoparticles with up to six times that of incident electric field and up to seventeen times at the interface between the particles. This shows that strong localized field is generated below the diffraction limit.

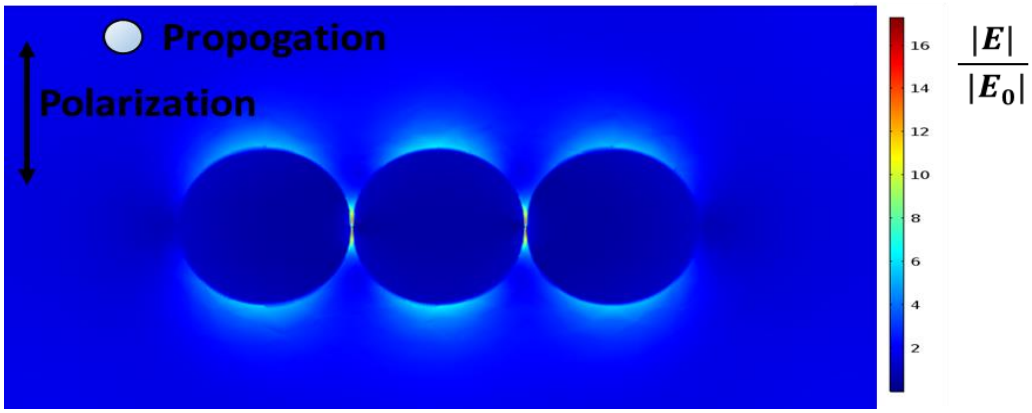

Figure 2. Top View of Electric Field Enhancement of Case 1 for d=0 and λ=532 nm

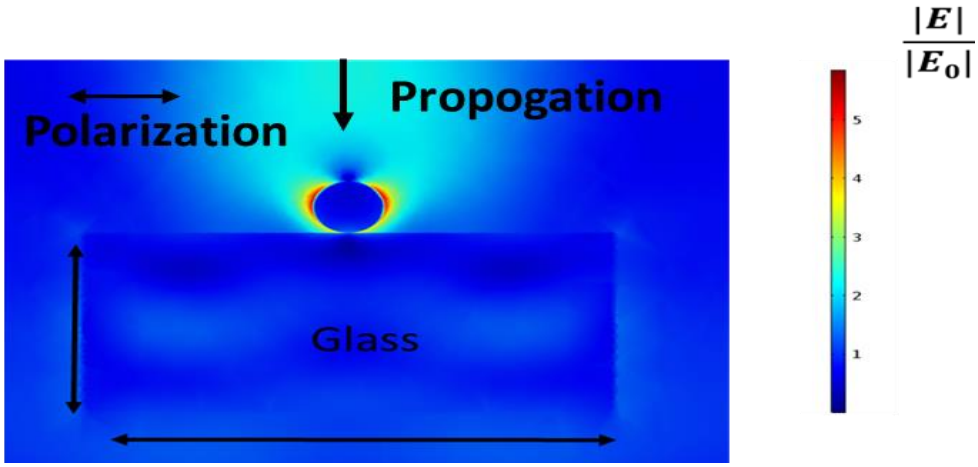

Figure 3. Side View of Fig 2.

Fig 4. illustrates the linear (Case 1) configuration in which the distance between the particles are varied from 10 nm to 50 nm. It can be seen that the plasmonic effects are observed only on the polarization direction and up to 6 times of that incident electric field.

Fig. 5 depicts the triangular (Case2) configuration when d=0. It is noticed that the electric field is enhanced up to 120 times between the adjacent nanoparticles, which is around 7 times higher than the linear configuration when d=0. We also observed that the maximum enhancement occur between the adjacent nanoparticles and due to the polarization direction we don't see the enhancement between the two adjacent nanoparticles which is located at the bottom of the figure in Fig. 5. Also, we see the plasmonic effect is on the direction of the polarization on the particles.

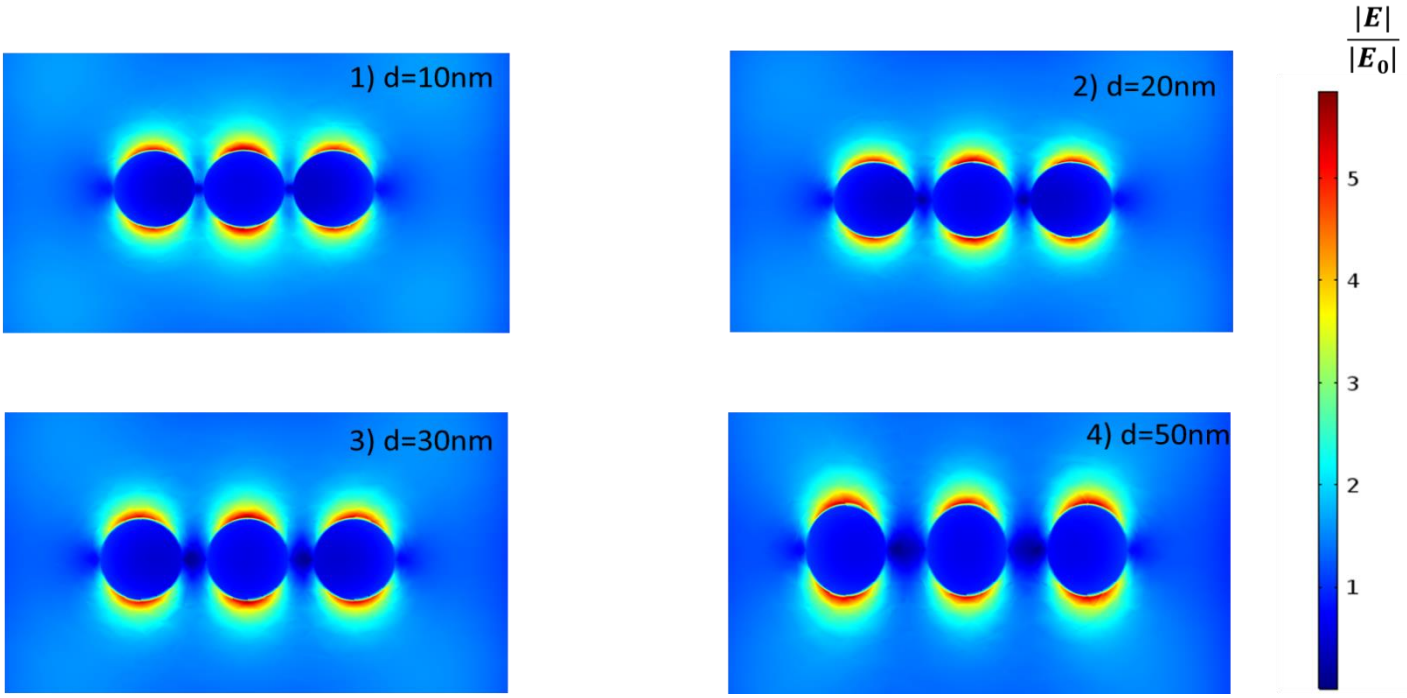

Figure 4. Electric Field Enhancement of Case 1 with varying *d*

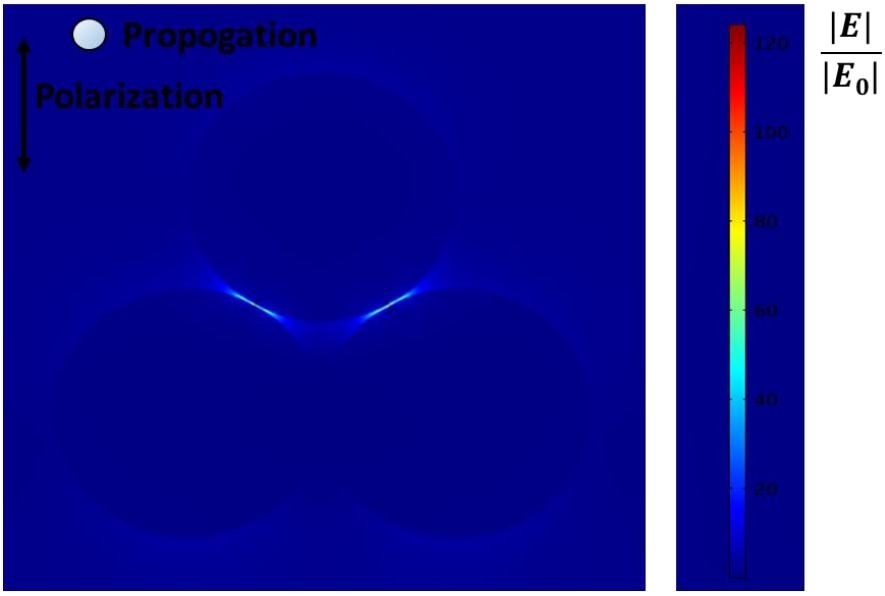

Figure 5. Electric Field Enhancement of Case 2 for *d*=0

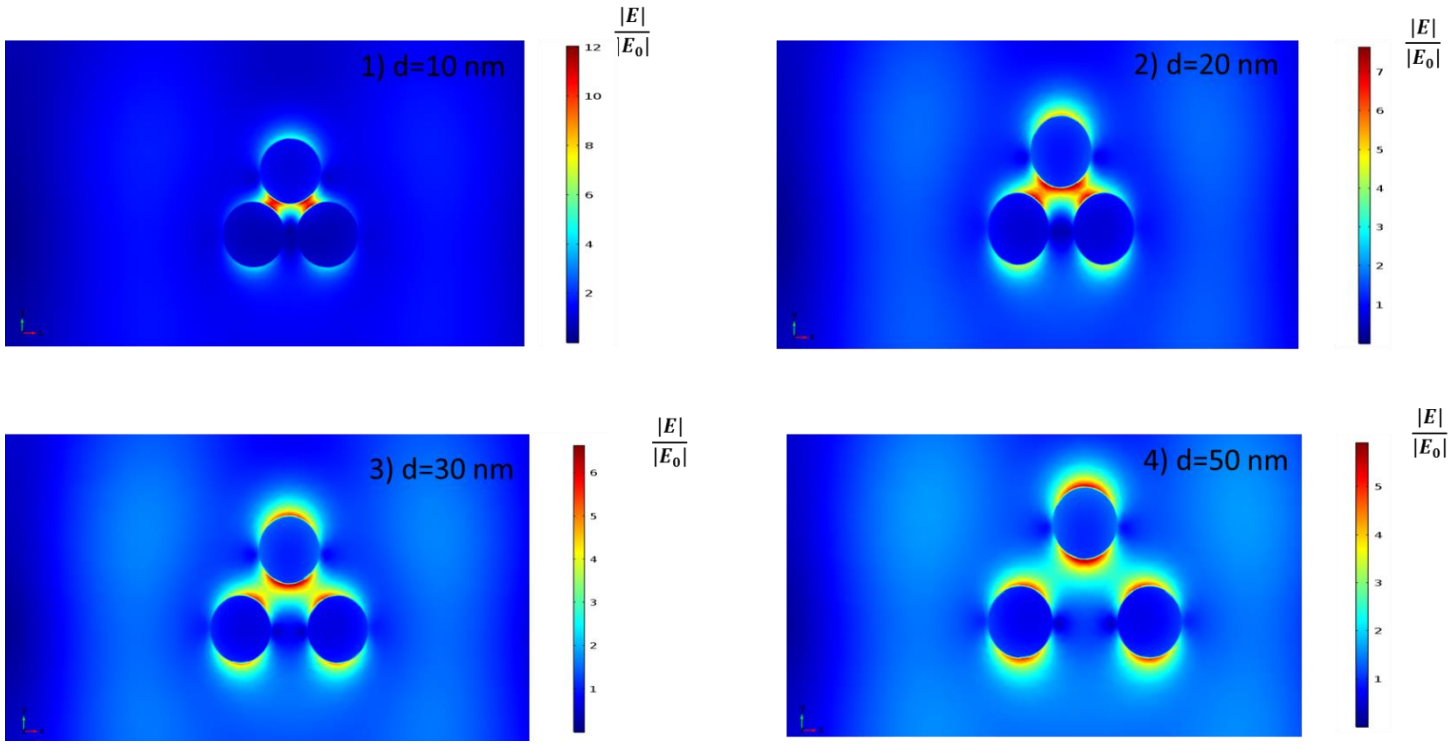

Figure 6. Electric Field Enhancement of Case 2 with varying *d*

Fig. 6 illustrates the electric field enhancement with varying *d* from 10 nm to 50 nm. It can be seen that the localized field enhancement is up to 12 times when *d* is 10 nm. Moreover, the surface plasmon polariton is much stronger within the particles and show a narrow excitation between the nanoparticles. This localized enhacement is decreased to between 6 to 7 times when *d* is between 20 nm to 50 nm. Another interesting result is that strength of the near-field effect is shifting from the between of the particles to the surface of the particles when *d* is between 20 to 50 nm and at 50 nm the particles start to behave almost individually. Also, the plasmonic effect can be seen along the direction of the polarization only (TE polarized) when *d* is at 50 nm. This indicates that the light/nanostructure interaction is affected significantly for different distance values between the particles as well as different configurations. It can be observed that the enhanced field is always much higher for triangular configuration than the linear case when the particles form cluster which means when *d* is 0. This enhanced field drop significantly when the particles start to have some spacing between each other. This gives an insight that the energy transfer between the particles are affected significantly for different configurations when they are at cluster form or d=0. Another interesting observation is that when the particle's distance, *d* , is 50 nm, the field enhancement is almost the same for linear and triangular configuration which implies that particles start to lose their interaction between each other at the near-field regime and behave similarly for these configurations.

As the light is absorbed and scattered by the metallic nanoparticle at 532 nm wavelength, absorption and scattering crosssection is important to understand for two cases that we looked at and mentioned in the previous section. It can be seen from Fig. 7 that absorption increases with particle spacing for linear case; however, absorption starts to gradually decrease with spacing for triangular case. This can be explained as the interference of propagation around the triangle starts to be reflected at the triangle corners. We can also see that at large spacing; the particles act more as individual particles and the results converge.

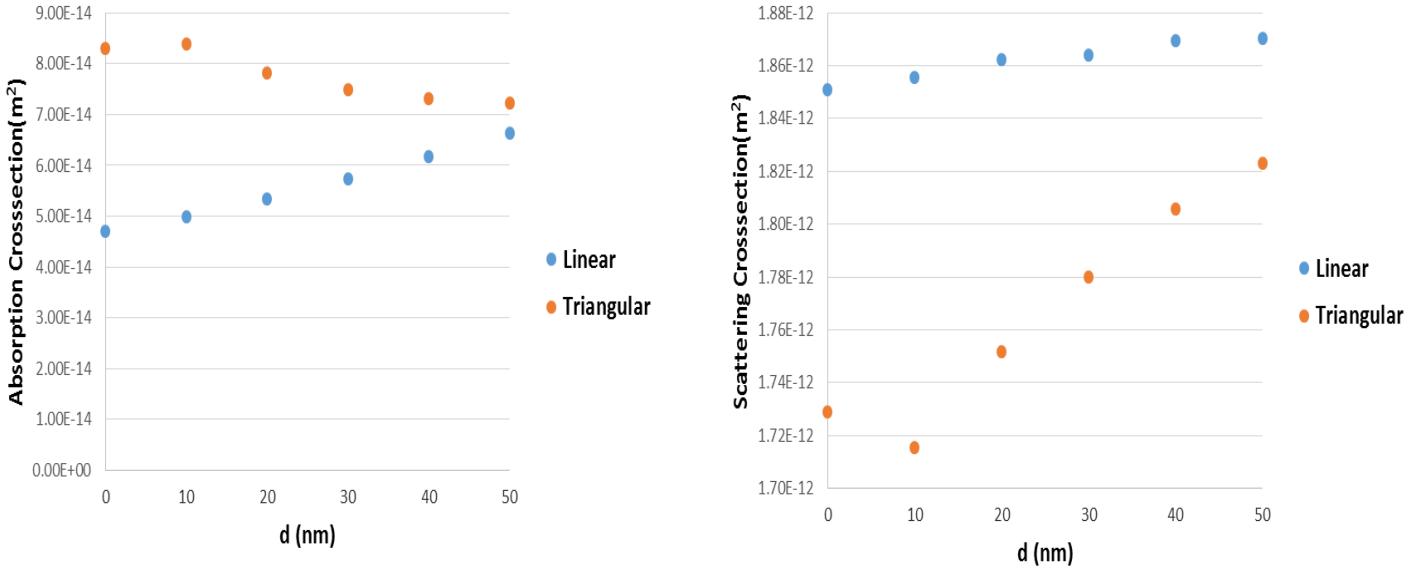

Figure 7. Absorption and Scattering Crosssection (m^2) versus particle spacing (*d*)

Also, we can see that scattering increases with particle spacing for both cases. This increase is linear for case 1 which is linear configuration. For case 2 which is the triangular configuration, interference between background and a resonant scattering results in asymmetric line shape or Fano type resonance. This phenomena is caused by the interference between two scattering amplitudes within the background and the resonant process. Indeed, this effect is observed when *d* is between 0-10 nm in which the near-field energy is localized and create an almost coherent excitation.

Fig. 8 shows the extinction crosssection which is the summation of absorption and scattering crosssection. It can be seen that scattering is more dominant over absorption at 100 nm of copper nanoparticle when interacts with 532 nm of wavelength and TE polarized light and thus the extinction crosssection is characterized by mostly scattering effect. We can also see that the two cases converge at the large particle spacing.

As it can be seen that the absorption crosssection is always higher for triangular case than the linear configuration. Moreover, scattering crosssection is higher for linear case. This also shows that 532 nm of wavelength and TE polarized light does not penetrate as far into the linear configuration compared to the triangular configuration. This implies that how far the energy is penetrated through the nanoparticles which affects the depth of the sintering in

the powder bed. Similarly, the closer the particles are together, the less light propagates into the powder bed which also affects the sintering depth.

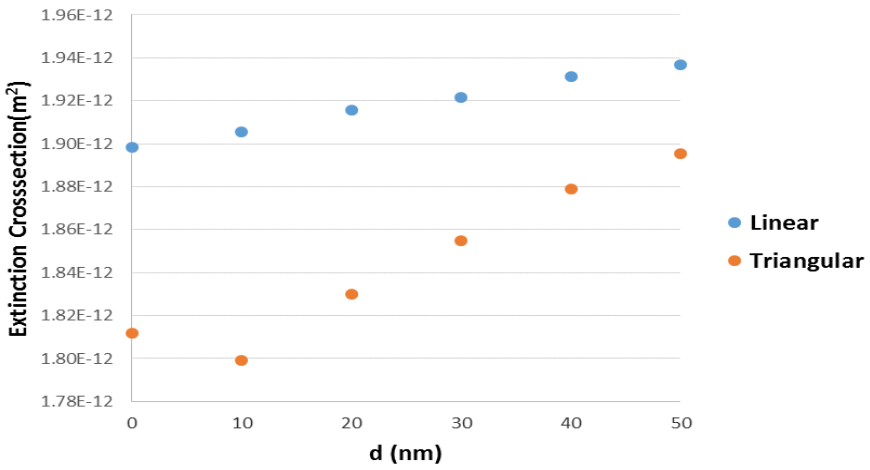

Figure 8. Extinction Crosssection (m^2) versus particle spacing (*d*)

4. Conclusion

We have shown that solutions of Maxwell's equation in frequency domain can depict the ability of near-field enhancement which results in surface plasmon generation below the diffraction limit. We examined the spacing effect between the nanoparticles with linear and triangular configurations for this behavior and observed the field enhancement to be highly dependent on the nanoparticle configuration. It is observed that nanoparticles when they are in a cluster group; in other words, when they are all touching each other, the maximum enhancement is achieved compared to the cases where there is a gap between the particles. The thermal radiation properties are nonlinearly characterized from 0-10 nm regime due to the strong and non-local near-field interaction between the particles with the linear and triangular configuration cases analyzed in this study. That shows that the light interaction with nanoparticles can be tuned by analyzing different configurations and the optimum configuration could be satisfied to achieve desired thermal radiation parameters to understand the sub-wavelength energy transport. Based upon the modeling and the experimental observations, it can be summarized that copper nanoparticles are a potential plasmonic waveguide and a step toward to understand photonic sintering between the particles for sub-wavelength 3D interconnects.

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