Modeling Co-Assembly of Binary Non-Monodispersed Nanospheres

Saurav Mohanty*, I-Te Chen, and Chih-Hao Chang

Walker Department of Mechanical Engineering, The University of Texas at Austin, TX 78712, USA

Colloidal nanoparticles have attracted significant interest as a viable approach to "bottom-up" nanofabrication. In such systems a monolayer of monodispersed nanospheres can achieve hexagonal close packing and be used as a lift-off or etching mask for lithography. Traditional self-assembly of colloidal nanoparticles have been extensively studied due to their applications in plasmonics and nanophotonics [1]. Another potential area is light extraction in solid-state lighting, where photonic crystals with single periodicity have been studied. However, they exhibit wavelength and angle sensitive behavior which is not ideal for broad range applications [2]. On the other hand, random surface roughening is difficult to design and are known to exhibit a broad periodic range [3]. To find a middle ground, nanostructures with dual periodicity have been studied to realize broadband light extraction in OLEDs with high efficiency enhancement but these nanostructures are expensive to fabricate [4]. Nanostructures with dual periodicity can be fabricated using colloidal assemblies with random distribution of binary particles. The main challenge for this approach is that there are presently no scalable methods for modeling and fabricating binary assemblies.

In this work, a geometric model was developed using line-by-line assembly of non-monodispersed binary nanoparticles to obtain a randomly closed packed assembly structure. Implemented in Matlab, the script initially accepts the diameter of the particle (d_1, d_2), image size, size variation and number ratio of particles as input variables, as illustrated in Figure 1. A matrix of the radii is formed based on the number ratio of particles sizes d_1 and d_2 with a standard deviation (σ). An average packing ratio of ~80% was obtained for 350 and 500 nm binary assembly with a size variation of 15%. To validate the results from the script, a binary nanoparticle assembly was experimentally fabricated. Polystyrene particles with combinations of 390-500 nm, 350-500 nm and 350-390 nm were mixed in different ratios of 1:1, 1:3 and 3:1. The mixture was then sonicated to obtain a uniform dispersion and then transfer coated onto a substrate. Using SEM images, the spatial-frequency spectra of the experimental assembly were then analyzed based on their intensity distribution of the rings using Fast-Fourier Transform (FFT). The peak frequencies of the FFT seem to match up well between the experimental and simulated model which validates the accuracy of the model. Based on this model we can design the particle diameters required to obtain the desired light extraction bandwidth. This work can find many applications in further improving the efficiency of light extraction devices. Future work remains to study the light extraction potential using binary assembly of nanoparticles by understanding the appropriate particle size distribution.

**saurav@utexas.edu*

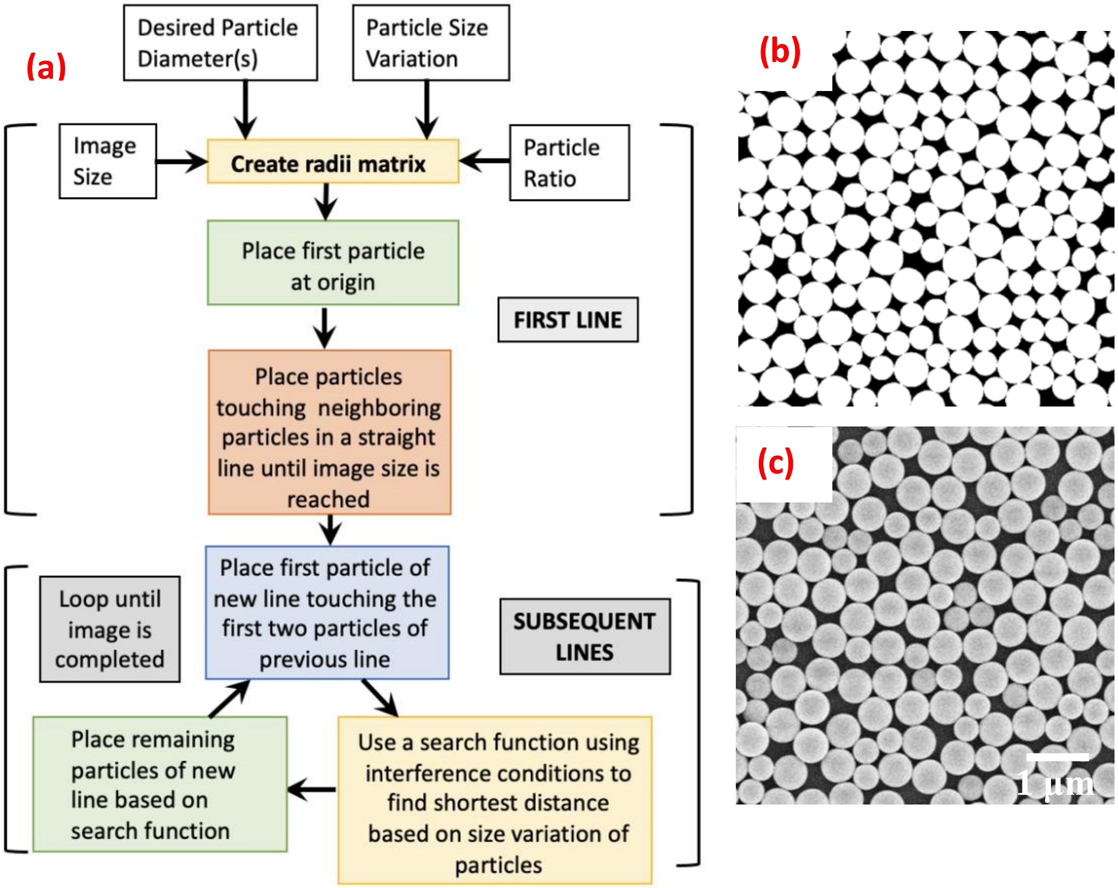

Fig. 1: (a) Flowchart of assembly algorithm; (b) Simulated binary assembly and (c) Experimental SEM image.

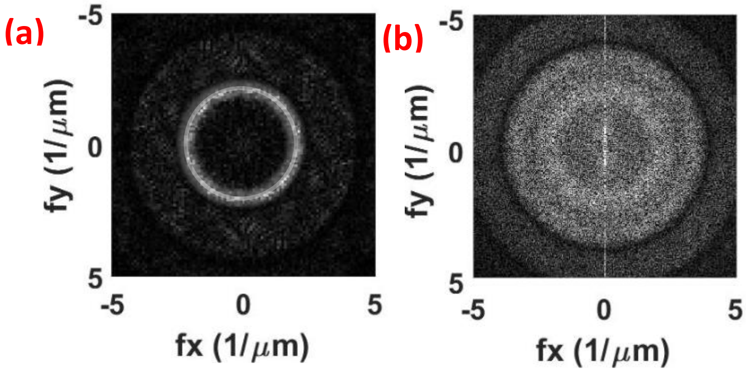

Fig. 2: Calculated 2D FFT spectra of (a) polycrystal assembly with monodispersed and (b) binary assembly.

REFERENCES

[1] J. C. Hulteen et al., Journal of Vacuum Science &. Technology A, vol. 13, no. 3, 1995.
[2] J.-G. Kim, et al. Optics. Express, OE, vol. 23, no. 17, pp. 22730–22739, Aug. 2015.
[3] Fujii, T., et al. Applied physics letters 84.6 (2004): 855-857.
[4] Bi, Yan-Gang, et al. Advanced Materials 25.48 (2013): 6969-6974.