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Effect of size dispersion on the lattice parameters of two-dimensional particle arrays: A possible uncertainty source in AFM size measurement of monodisperse particles

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Atomic force microscopy (AFM) is a possible candidate for an accurate method of sizing monodisperse particles for developing nanoparticle size standards (APEC ISTWG Project, 2006). In the AFM method, monodisperse particles such as polystyrene latex spheres are arranged in a two-dimensional closed pack array on a solid surface, and the average particle diameter is determined by measuring the lattice parameter. A systematic bias in the measurement may occur due to the size dispersion of the particles, but this effect has not been studied in detail so far. In the present study, a theoretical simulation of particle arrangement in a two dimensional array was carried out to investigate this effect.

In the simulation, seventy-two particles sampled randomly from a normal size distribution with mean diameter 100 nm and a standard deviation σ were placed onto a $2000\,\mathrm{nm} \times 2000\,\mathrm{nm}$ area. The values of σ were set at 0, 2, 4, and 8 nm. The Markov chain Monte Carlo method was employed to determine possible arrangements of the particles, with assuming that the interparticle potential is given by the sum of van der Waals potential and a hard core repulsive potential. Simulation was carried out more than five times for a specified value of σ.

Examples of particle arrangement obtained in this way are shown in Figure 1. The ideal closed packing is realized for σ = 0 nm, while a regular periodic structure is barely discernible for σ = 8 nm. In the intermediate cases of σ = 2 nm, and 4 nm, it is seen that a local regularity is retained.

For each pair of two adjacent particles *i* and *j*, the gap was calculated from

$$g_{ij} = l_{ij} - (D_i + D_j)/2\,, \qquad (1)$$

where l_{ij} is the distance between the centre of the particles, and D_i and D_j are the particle diameters. It is found that except for the case of σ = 0 nm, particles in approximately 75 to 80 % pairs are in direct contact (i.e., $g_{ij} = 0$) irrespective of the value of σ. Considering the finite resolution of AFM images, we may assume that in practical AFM measurements the mean particle diameter is determined from

$$\overline{D} = \sum_{(g_{ij} \le g)} l_{ij} \Big/ \sum_{(g_{ij} \le g)} 1\,, \qquad (2)$$

where g represents a threshold gap indicating that pairs with $g_{ij} > g$ are excluded from measurement.

Figure 2 shows $\overline{D}$ as a function of g. Even for g = 0, a bias in $\overline{D}$ is observed. This occurs because larger particles have higher probability of having adjacent particles in direct contact than smaller particles. Because a sizing error in the order of 0.5 % is considered not negligible in developing particle size standards, the result shown in Figure 2 indicates that the size dispersion can be a non-negligible uncertainty source in particle sizing by AFM.

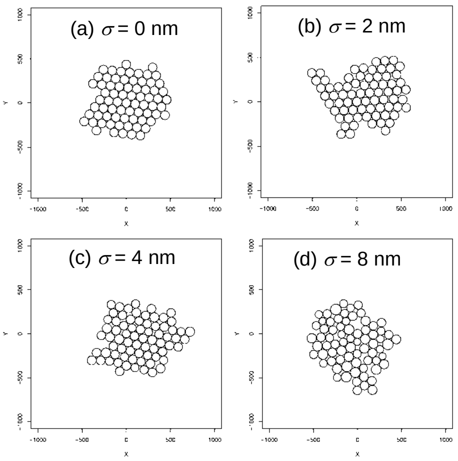

Figure 1. Typical two dimensional arrangements of 100 nm nearly-monodisperse particles with (a) σ = 0 nm, (b) 2 nm, (c) 4 nm, and (d) 8 nm.

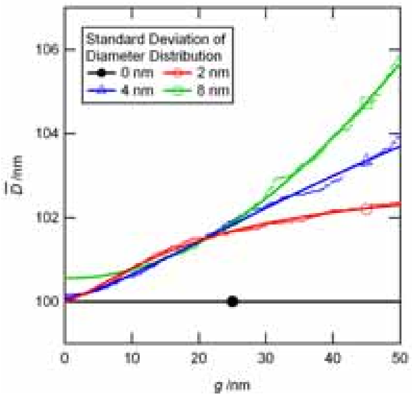

Figure 2. Average diameter $\overline{D}$ as a function of the resolution limit g.

APEC ISTWG Project (2006), *Interlaboratory Comparison on Nanoparticle Size Characterization*, Report on measurement results.