

Polymer photonic crystal band-gap modulation using PbS quantum dots

Aurel Diacon^a, Edina Rusen^{a,*}, Alexandra Mocanu^a, Leona Cristina Nistor^b

^aUniversity Politehnica of Bucharest, Department of Polymer Science, 149 Calea Victoriei,
RO-010072 Bucharest, Romania

^bNational Institute of Materials and Physics, 105 bis Atomistilor, 077125 Magurele-Ilfov, Romania

Supplementary file

The reviewers comment was particularly welcome giving us the opportunity to demonstrate mathematically the band gap modulation for the different systems. Therefore, the next reasoning is presented as follows:

For the system A

$$\left. \begin{array}{l} \lambda = n_{\text{eff}} \cdot 1.632 \cdot d \\ \lambda = 540nm \\ d = 208nm \end{array} \right\} n_{\text{eff}} = 1.59$$

$$n_{\text{eff}} = f \cdot n_{\text{ST-AA}} + 1 - f \quad (1)$$

$$n_{\text{air}}=1$$

- the AFM (FFT) analysis of the particles arrangement confirmed the FCC structure, thus the packing factor is $f=0.74$;

From the equation 1 the value of $n_{\text{ST-AA}}$ is 1.797.

For the system D

For the system D, the refractive index value can be approximated with the value of $n_{\text{ST-AA}}$, or slightly increased, considering the small quantity of particles represented by the PbS incomplete shell.

$$\left. \begin{array}{l} \lambda = n_{\text{eff}} \cdot 1.632 \cdot d \\ \lambda = 510nm \\ d = 226nm \end{array} \right\} n_{\text{eff}} = 1.382$$

$$n_{eff} = f \cdot n_{ST-AA} + 1 - f \quad \Longrightarrow \quad f=0.48$$

The value obtained for the packing factor could be explained as an average of the fraction of space occupied by spheres. The fraction occupied by the spheres determines the fraction of air. Thus, the air fraction represents a consequence of the particles arrangement, which is put into evidence in the next figure with red squares. A disruption of the FCC structure is clearly visible.

