Electronic Supplementary Material (ESI) for CrystEngComm.

Muscovite Mica as a Growth Template of $PC_{61}BM$ Crystallites for Organic Photovoltaics

Jon Feenstra, Maarten van Eerden, Alexander K. Lemmens, Wester de Poel, Paul H.J. Kouwer, Alan E. Rowan, John J. Schermer

Supplementary information

1. Molecular structures of $PC_{61}BM$ and P3HT.

a b

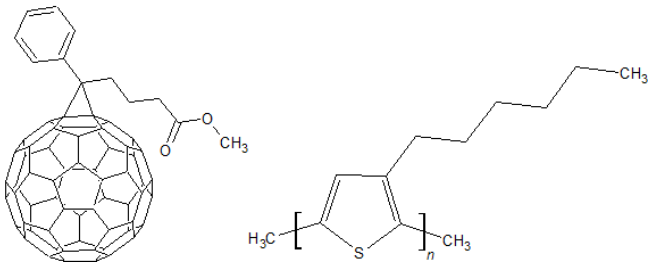

Figure 1: Molecular structures of $PC_{61}BM$ (a) and P3HT (b).

2. AFM analysis

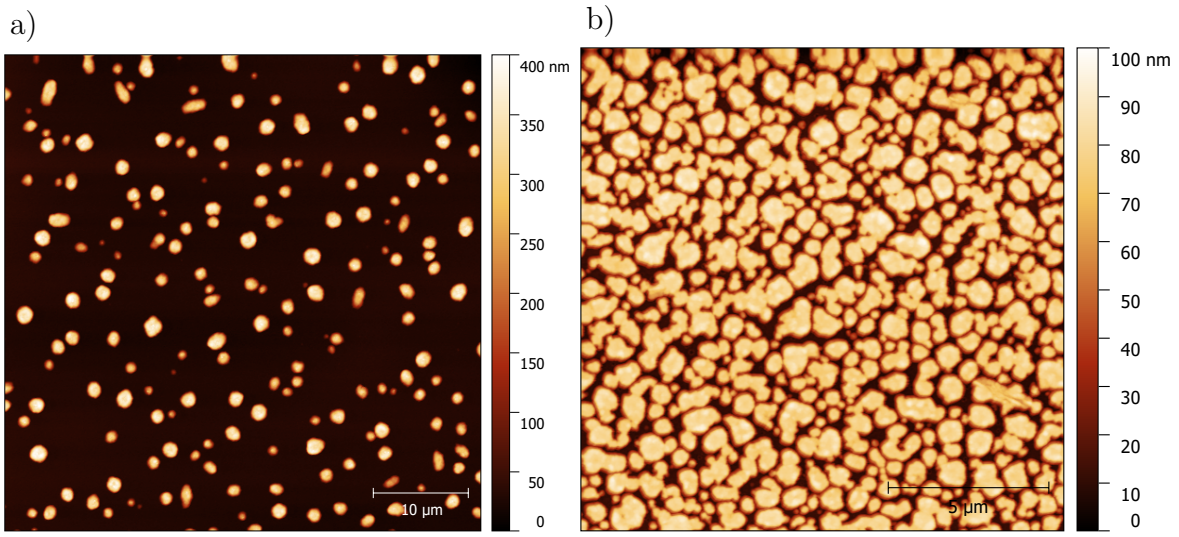

Figure 2: (a) AFM image showing the morphology of an active layer on mica obtained from an $R = 1$ blend ($T = 140\,^{\circ}C$). The average crystallite diameter obtained from two AFM images of this sample is 1.2 µm which shows good agreement with the value obtained from optical Phase Contrast Microscopy (PCM) images shown in Figure 4a, justifying our approach to use PCM images to determine the crystallite characteristics. (b) AFM image showing the morphology of an active layer on mica obtained from an $R = 5$ blend ($T = 140\,^{\circ}C$). Average crystallite diameter and nucleus density corresponding to these processing parameters are shown in Figure 4c of the main manuscript.

3. Nature of $PC_{61}BM$ crystallization on muscovite mica

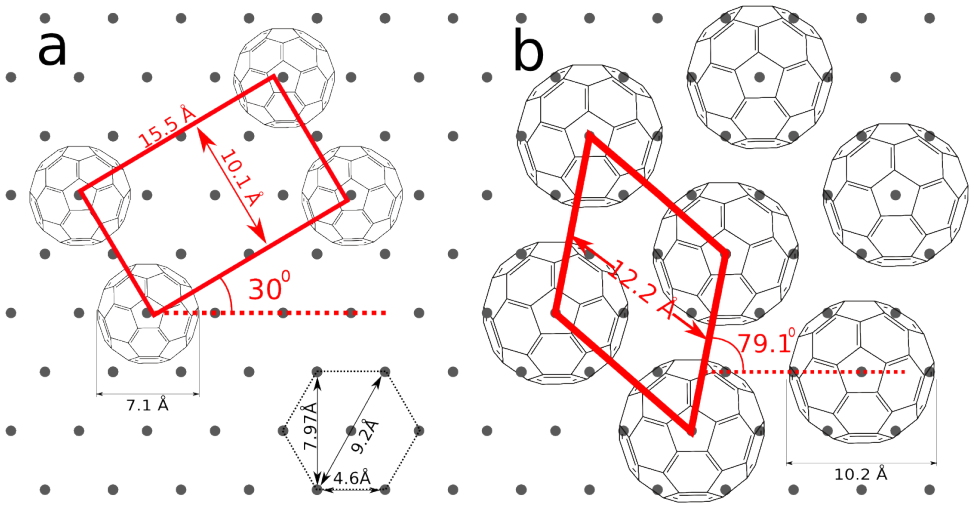

Figure 3: Schematic representation of the (001)-plane of Muscovite mica showing hexagonal symmetry of the surface oxygen-atoms. The relation between $PC_{61}BM$ (funtionalisation not shown for clarity reasons) and the mica template is shown for two cases. The a-distorted cubic lattice (a) proposed by Li et al.[1] using the nucleus-to-nucleus diameter (7.1 Å) for the Buckminsterfullerene in $PC_{61}BM$, and the hexagonal structure (b) proposed in the current study in which the Van Der Waals diameter (10.2 Å) for the Buckminsterfullerene is considered. Lattice parameters are shown in red and the dimensions of a single hexagon are indicated.

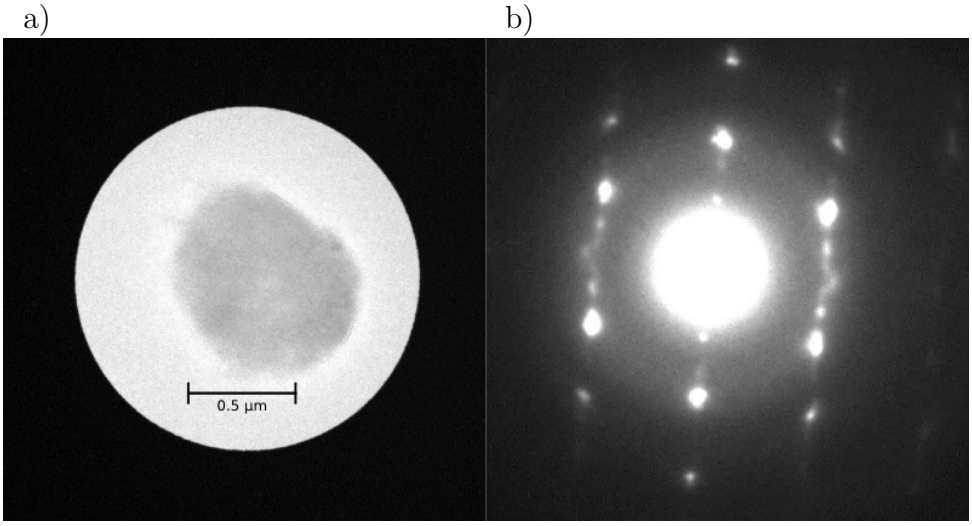

Figure 4: Transmission Electron Microscopy image (a) and diffraction pattern (b) of a single $PC_{61}BM$ crystal ($R = 1$, $T = 140\,^{\circ}C$). For TEM sample preparation the layer was transferred from mica to a TEM mesh grid.

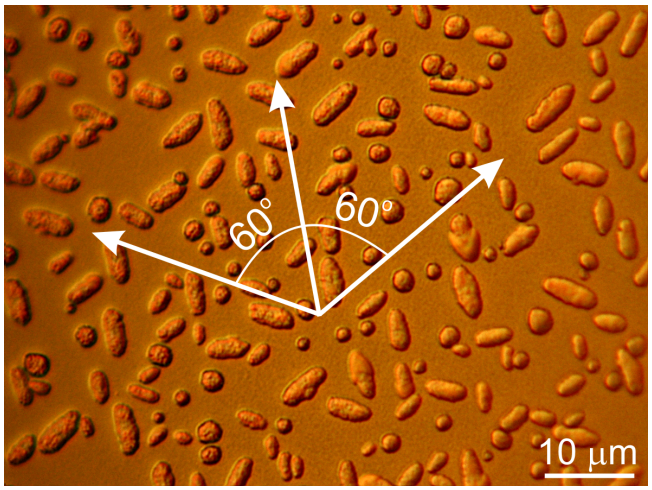

Figure 5: PCM image showing the morphology of an active layer on mica obtained from an $R = 1$ blend with a total concentration of 40 mg mL^{-1} ($T = 140\,^{\circ}C$). The long axes of the elongated crystallites show a 60 °orientation with respect to each other, adopting the symmetry of the underlying hexagonal muscovite mica substrate, which is a distinct feature of epitaxial crystallisation.

4. Influence of P3HT regioregularity on $PC_{61}BM$ crystallisation

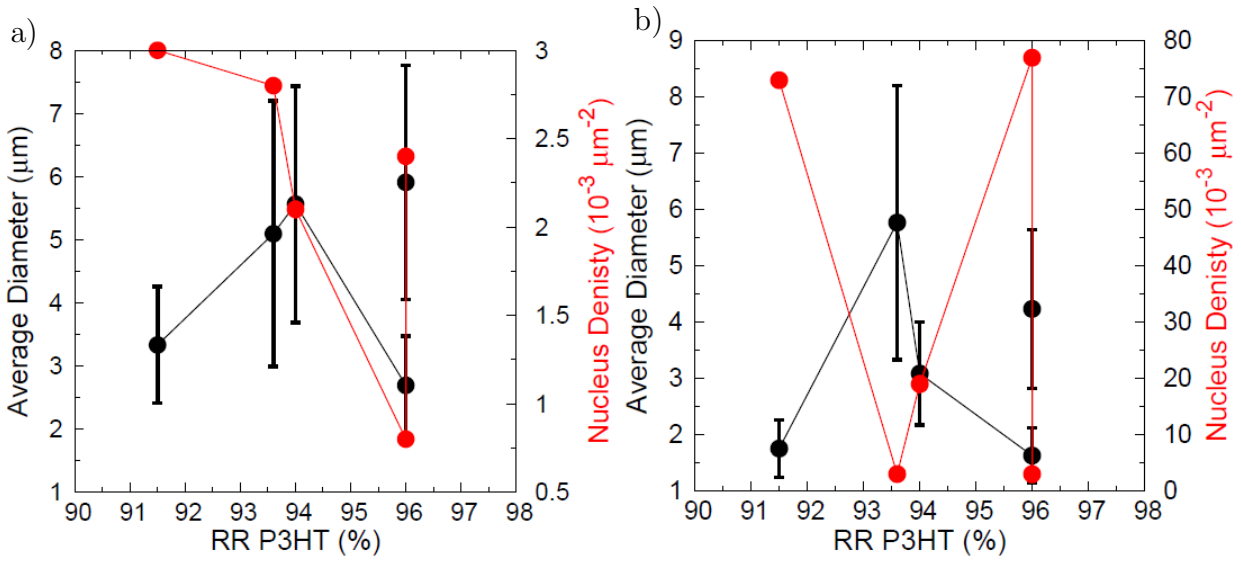

Figure 6: Average particle diameter and nucleus density of $PC_{61}BM$ crystallites as a function of the regioregularity (RR) of P3HT from samples produced on glass (a) and mica (b). The $PC_{61}BM$:P3HT ratio was 1:1, the annealing time and temperature were 30 minutes and 140 °C , respectively and M_w^{P3HT} was 37 kDa for all samples except the sample produced using P3HT with an RR of 93.6%, for which M_w^{P3HT} was 31 kDa. The RR of P3HT strongly influences the crystallisation of P3HT and can thereby also impact the diffusion, nucleation and crystallisation of $PC_{61}BM$, as was elaborated in the main text. However, the nucleation and crystallisation of $PC_{61}BM$ from the different $PC_{61}BM$:P3HT blends studied here cannot be directly correlated to the RR of P3HT. For example, the two highest nucleus densities on mica are obtained for the lowest and highest RR. Moreover, two batches of P3HT with identical RR and identical M_w^{P3HT} (96% and 37 kDa, respectively), yield very different nucleus densities and average particle diameters. This implies that other P3HT properties than the RR and Mw are playing a significant role in the crystallisation of $PC_{61}BM$. These might include the polydispersity (which is the ratio of the weight- and number-averaged molecular weight) and purity of P3HT, which are however beyond the scope of this research.

References

1 L. Li, G. Lu, S. Li, H. Tang and X. Yang, *The Journal of Physical Chemistry B*, 2008, **112**, 15651 - 15658 .