

Characterization of Cross Sectional Profile of Epitaxially Assembled Block Copolymer Domains using Transmission Small Angle X-Ray Scattering

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Abstract: Transmission small angle X-ray scattering (tSAXS) was used to characterize the cross section of poly(styrene-*b*-methyl methacrylate) block copolymer line gratings assembled on chemically templated substrates with a pitch less than 50 nm. X-ray diffraction data covered a broad Q_x and Q_z region were collected and analyzed, where the x-axis denotes the in-plane direction perpendicular to the line gratings and z-axis is along the thickness direction. The X-ray data can best be fitted with a cross section comprised with both footing and top rounding. The simplest model to simulate a cross section with both footing and top rounding is a stack of three trapezoids, each with discrete side wall angle, height and width. Even with this simple 3-trapezoidal model there exist seven fitting parameters, however, there also exist sufficient X-ray data to ensure a fit with a reasonable quality. Figure 1 illustrates this point; the 7-parameter model was determined by simultaneously fitting all five diffraction curves at 5 discrete Q_x. The best fitted cross section of PS-PMMA block copolymer nanopatterns is given in Figure 2. It is noteworthy that the area occupied by each component of the nanopatterns is exact 50% in consistent with the composition of the copolymer used. This observation further highlights the accuracy of the X-ray data and its analysis. The line edge roughness (1σ) was also determined by the intensity decay rate along Q_x, known as apparent Debye-Waller factor. The cross section and the interface roughness value obtained from X-ray data will be discussed and compared with computer simulation results.

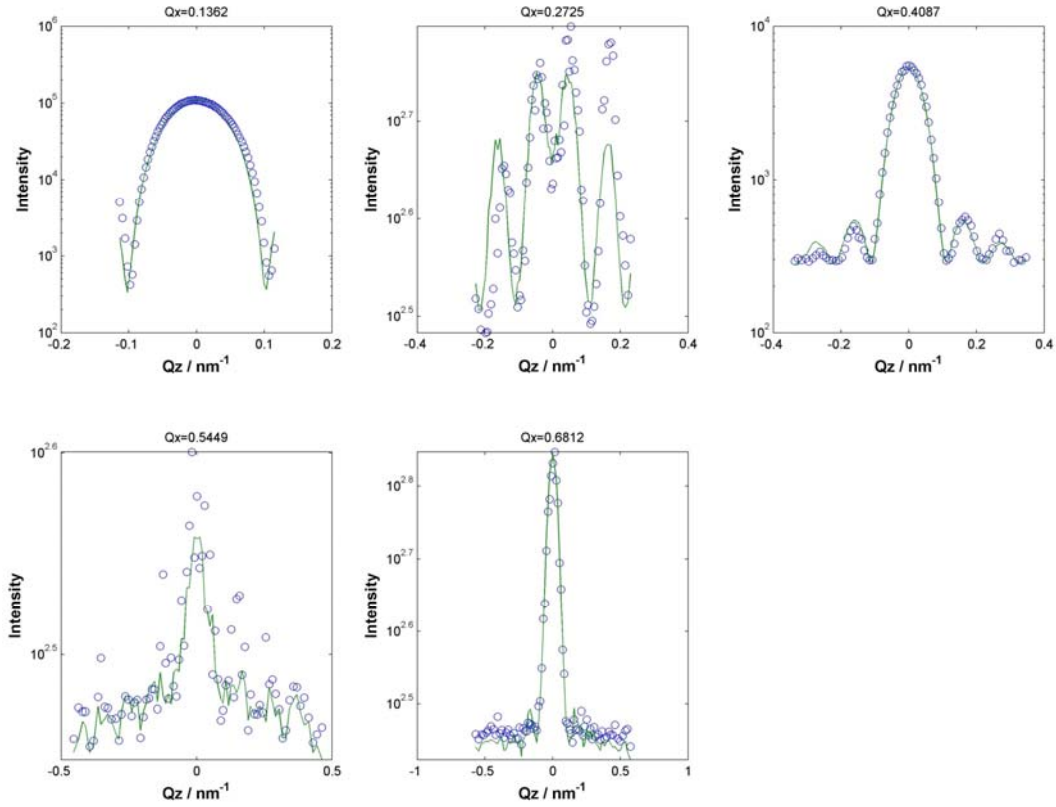


Figure 1: A simultaneous non-linear least square fitting of scattering intensity versus Q_z at different given Q_x . A model of a stack of three trapezoids gave significant lower χ^2 than a model of mono trapezoid.

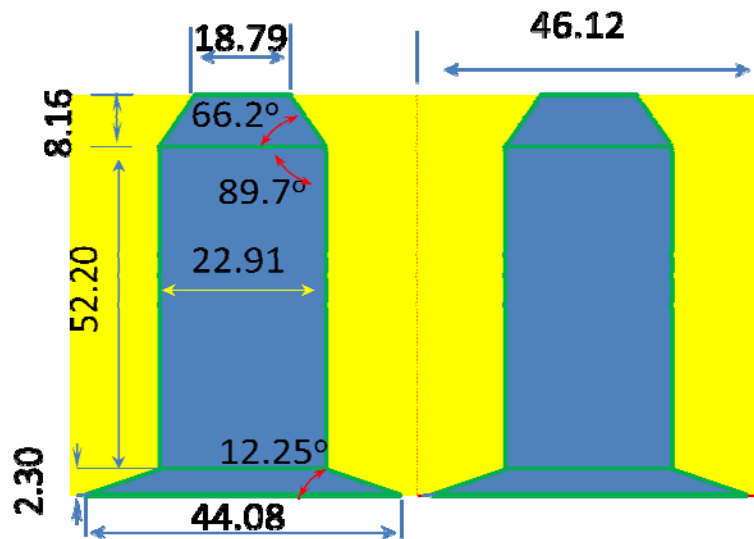


Figure 2. Illustration of cross sectional profile of block copolymer domains assembled on an epitaxial template. The yellow part is poly(methyl methacrylate), while the blue part if polystyrene.