Structure of grain boundaries in a layer-stacked 2D polymer

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Two-dimensional (2D) polymers hold great promise in the rational materials design tailored for next-generation applications. However, little is known about the grain boundaries in 2D polymers, not to mention their formation mechanisms and potential influences on the material's functionalities. Using aberration-corrected high-resolution transmission electron microscopy, supported by quantum chemical calculations, we presented a direct observation of the grain boundaries in a layer-stacked 2D polyimine with a resolution of 2.3 Å [1]. We found that the polyimine growth followed a "birth-and-spread" mechanism. Antiphase boundaries implemented a self-correction to the missing-linker and missing-node defects, and tilt boundaries were formed. Notably, we identified grain boundary reconstructions featuring closed rings at tilt boundaries. This contribution focuses mainly on the character of the reconstructed grain boundaries, which we have characterized using quantum chemical calculations. These revealed that boundary reconstruction is energetically allowed and can be generalized into different 2D polymer systems. We envisage that these results may open up the opportunity for future investigations on defect-property correlations in 2D polymers.

References

[1] Qi, H.; Sahabudeen, H.; Liang, B.; Položij, M., Addicoat, M.A.; Gorelik, T.E.; Hambsch, M.; Mundszinger, M.; Park, S.; Lotsch, B.V.; Mannsfeld, S.C.B.; Zheng, Z.; Dong, R.; Heine, T.; Feng, X.; Kaiser, U., Science Advances 6 (2020), eabb5976.

Figures

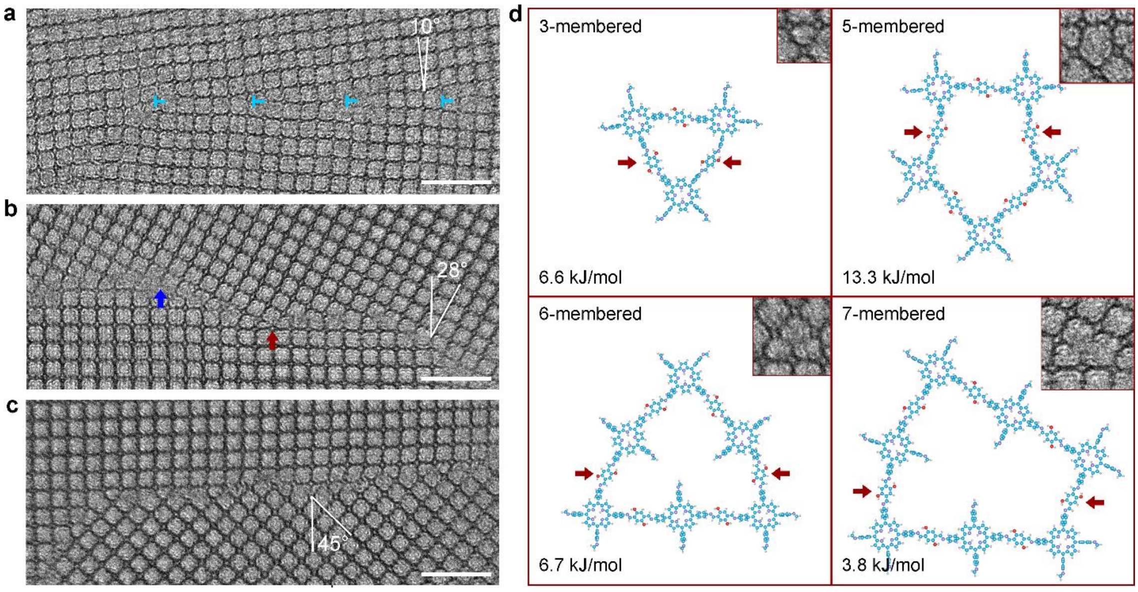

Figure 1: Low-angle and high-angle grain boundaries visualized by AC-HRTEM imaging and atomic models of the novel grain boundary structures