High-resolution XRD characterization of surface guided Xanthine derivatives for optical metamaterial application

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Numerous biological organisms employ template-assisted crystallization of molecular solids to produce crystal morphologies with unique optical properties that are difficult to reproduce synthetically. Here, we report the growth of large, bio-inspired, birefringent, and defect-free crystalline sheets of a xanthine derivative (theophylline), reaching several millimeters in length, on a single-crystal (11–20) quartz template. Structural mismatch between the hexagonal quartz substrate and the orthorhombic theophylline layer leads to distinctive form of heteroepitaxy.

The surface-guided growth of theophylline crystalline sheets is characterized by a well-defined orientation both in-plane and out-of-plane with respect to the substrate, resulting in pronounced optical anisotropy parallel to the quartz surface.

A combination of out-of-plane and in-plane X-ray diffraction measurements, performed using a Rigaku SmartLab diffractometer, reveals lattice matching between the planes perpendicular to substrate surface, namely (−2204) of quartz and the (017) of theophylline. Molecular-level simulations of interfacial bonding highlight the critical role of hydrogen bonds in establishing coherence between the quartz substrate and the theophylline layer. High-resolution in-plane measurements also confirm the angular relationship between the slow optical axis of the film, [002], and slow optical axis of quartz, [1-100].

This study demonstrates an unusual heteroepitaxial relationship between quartz and an organic dielectric film and highlights the power of combining in-plane and out-of-plane high-resolution X-ray diffraction techniques to elucidate structural features of optically anisotropic materials.

A. Niazov-Elkan, M. Shepelenko, L. Alus, M. Kazes, L. Houben, K. Rechav, G. Leitus, A. Kossoy, Y. Feldman, L. Kronik, P. G. Vekilov, D. Oron. Advanced Materials (2024) 36, 2306996