

Structure of Protein Cage Supercrystals Revealed by Angular X-ray Cross-Correlation Analysis

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Biohybrid supercrystals are highly ordered 3D assemblies of protein nanocages, offering versatile structural designs through the selection of protein nanocages and their ability to encapsulate various cargos within their cavities. By loading nanoparticles into these nanocages, diverse and complex superstructures can be engineered. In this study, individual biohybrid supercrystals are investigated using small-angle X-ray diffraction. As the samples may consist from single to several crystalline grains, angular X-ray cross-correlation analysis is used to analyze the angular correlations within the intensity distribution in 3D reciprocal space, enabling the determination of the unit cell parameters of the superlattice. Encapsulated nanoparticles serve as effective X-ray scattering markers, facilitating precise identification of the nanocage positions within the superlattice. The arrangement of nanoparticles in the unit cell is validated by comparing the experimental and calculated radial intensity profiles. The findings confirm the superlattice structures of unitary protein-nanoparticle composites, binary composites (including homobinary and heterobinary designs), and supercrystals with core-shell morphologies. Furthermore, single-grain and twin-domain structures are identified, demonstrating the capability of this technique for defect characterization and crystal engineering.