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Topological Defects in Polycrystalline Hexosomes from β-Cyclodextrin Fatty Esters

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Electronic Supplementary Information

Figure S1. Continued next page.



Figure S1. Cryo-TEM images of various polycrystalline facetted and tortuous β CD-C₁₄ particles. Tilt grain boundaries and dislocations in these particles have been described in the main manuscript (**Figures 5-7**).



Figure S2. TEM images of polycrystalline β CD-C₁₄ particles. After deposition of the suspension and air-drying, the grid was mounted in a Gatan 626 specimen holder and flash-frozen in liquid nitrogen before being transferred in the microscope. The preparation was observed under low dose conditions, at low temperature. The arrows point at regions corresponding to axial projections of the hexagonal columnar organization, exemplified by the inset in image a that corresponds to the framed region.



Figure S3. Definition of the tilt angle between two adjacent grains separated by a symmetrical tilt grain boundary. The rotation angle θ between two adjacent grains is defined as the smallest angle between (10) planes from each grain. Example of a $\Sigma = 7$ boundary with a tilt angle $\theta = 21.8^{\circ}$. The yellow and blue disks are columns with 7 and 5 neighboring columns, respectively.



Figure S4. Two-dimensional dichromatic patterns formed by rotating one elementary hexagonal lattice with respect to the other by the angle indicated in parentheses around one site common to both crystals. The elementary lattices are drawn with blue and red dots, respectively, and the unit cells of both lattices are indicated by blue and red rhombi. The coincidence site lattice (CSL), drawn with gray lines, is characterized by the coincidence index Σ defined by the ratio of the surface of the unit cell of the CSL (indicated by a gray rhombus) to that of one elementary lattice. All CSLs have been oriented so that one plane of maximum coincidence is vertical.



Figure S5. Two views of the cryo-TEM image of the stepped grain boundary analyzed in **Figure 5i-k**. The original image has been rotated to help visualize the tilt angle between the two grains and the local distortion of the lattice planes in the vicinity of the boundary (indicated by arrows). The images have been prepared using the free Blender software (www.blender.org).



Figure S6. Example of a stepped tilt grain boundary (GB) in a β CD-C₁₄ multidomain hexosome with a descriptive model of column organization. The black circles are projections of β CD-C₁₄ columns organized in a hexagonal structure. The yellow and blue disks are columns with 7 and 5 neighboring columns, respectively. The tilt angle measured between the adjacent grains is $25 \pm 1^{\circ}$. A larger view of the particle is shown in ESI **Figure S1g**.



Figure S7. Three views of the cryo-TEM image of the grain boundary and dislocation analyzed in **Figure 6**. The original image has been rotated to help visualize the tilt angle between the grains and the local distortion of the lattice planes in the vicinity of the boundary (indicated by the arrow) and edge dislocation (T). The images have been prepared using the free Blender software (www.blender.org).