Supporting Information

Complex Concaved Cuboctahedrons of Copper Sulfide Crystals with Highly Geometrical Symmetry Created by a Solution Process

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Experimental

Simulation synthesis of CuS in oil bath. For reaction in an oil bath, equivalent amounts of reagents were transferred into a 50 ml flask, which was sealed carefully. Then it was immersed into an oil bath at 140 °C. In about 10 min, the solid-state sulfur melted into yellow droplets. After half an hour, the color of the solution got dark gradually. The solution turned black suddenly after 70 min. The precipitated black product was collected by centrifugation of the mixture immediately, then washed with carbon disulfide and absolute ethanol for several times respectively and dried in a vacuum at 60 °C for 4 h. Several kinds of branched hexagons, such as individual hexagonal flakes, conjoined two or three flakes and some already perfectly scaffolded cuboctahedra were observed to coexist in the product.

After reaction for 4 h, a majority of particles are in a form of concaved cuboctahedron except for a few defaulted structures with incompletely branched features. Further observations indicated that each particle has an edge length of 0.5~1 μm and a thickness of 100 nm, which are a little smaller and thinner than those made in the autoclave.

Calculation of the dihedral angle. A perfect concaved cuboctahedron of CuS crystal is chosen as the model. θ shown in Figure S1 is the supplementary angle of a dihedral angle, which can be calculated by law of cosines $\cos \theta = \frac{a^2 + b^2 - c^2}{2ab}$. If the edge of the crystal is set as l , a and b will be $\frac{\sqrt{3}}{2}l$ and c will be $\sqrt{2}l$ respectively. θ value was calculated to be 109.5° . Then the correspondingly dihedral angle of the two planes is 70.5° .

Figure S1. Calculation of the dihedral angle of a concaved cuboctahedron crystal.