

Controlled Synthesis of Wurtzite CuInS₂ Nanocrystals and Their Side-by-Side Nanorod Assemblies

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Electronic Supplementary Information

S1. Crystal lattice structure

Normally, CuInS_2 has three crystalline forms: chalcopyrite, zinc blende and wurtzite. Chalcopyrite is common in natural CuInS_2 , which has a tetragonal unit cell. When Cu(I) and In(III) distributing equally in the cation sites of chalcopyrite CuInS_2 , the tetragonal cell could be simplified into cubic cell, that is zinc blende. In the wurtzite phase, sulfur ions are hexagonally close-packed, presenting a nearly fixed structure, while In(III) and Cu(I) are placed randomly through the tetrahedral interstices of the sulfur framework with same occupation possibility to meet the charge balance on the whole.

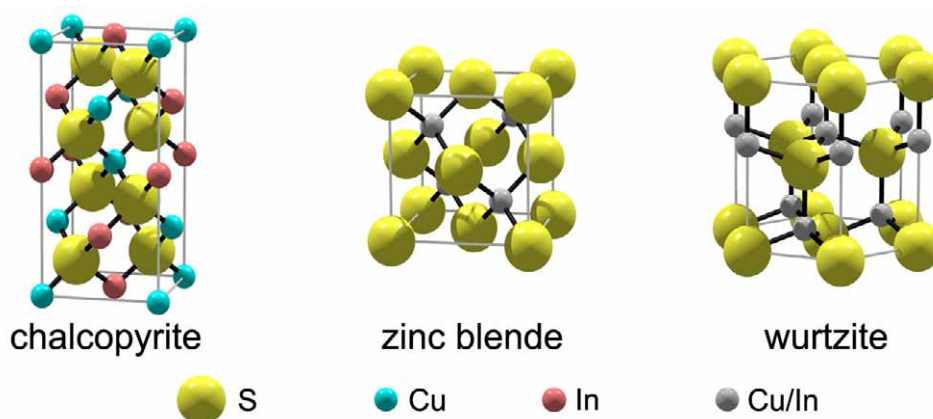


Fig. S1 Crystal structures of chalcopyrite, zinc blende and wurtzite CuInS_2 .

S2. Anneal Process

To test the stability, films of wurtzite CuInS₂ nanocrystals (sample III-2) were put into the furnaces undertaking the anneal process. Heat treatment is necessary in fabricating PV devices to remove the surfactants, which would enhance the performance of devices. The CuInS₂ film was annealed at 400 °C for 2 hours under N₂ flows. It is observed that no phase transition has happened. The XRD pattern could still be indexed as wurtzite CuInS₂ (**Fig. S2**).

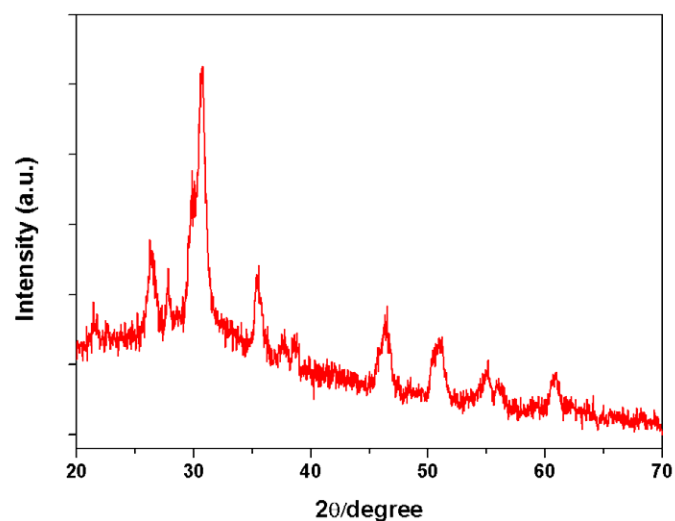


Fig. S2 XRD pattern of wurtzite CuInS₂ film after annealing

S3. Assemble Nanorods

The experimental setup in this section is extremely simple (**Fig. S3**). It is necessary to avoid shaking the experimental setup after putting the substrate to the container, but exposure to the air will not affect the arrangement of nanorods.

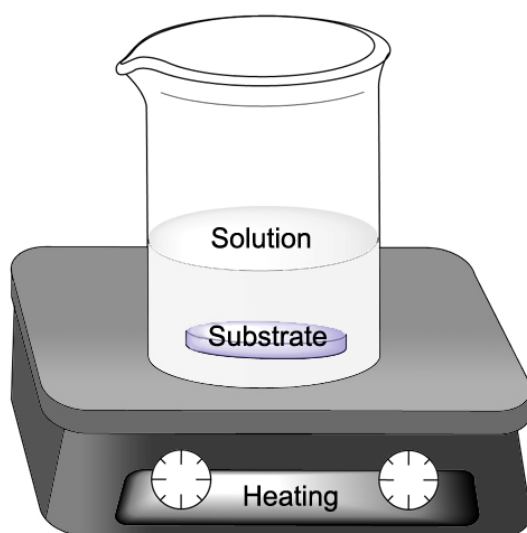


Fig. S3 Schematic diagram of the equipment.

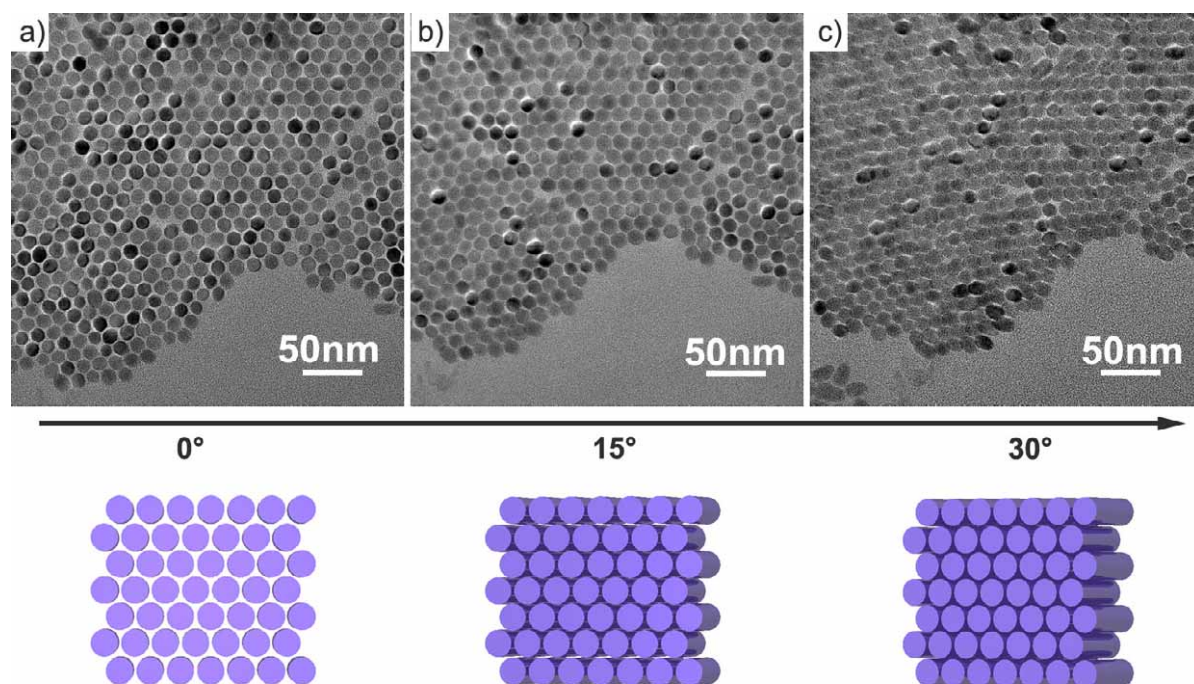


Fig. S4 (a)TEM images of perpendicularly aligned nanorods, (b)after tilted by 15°, (c)after tilted by 30°, and schematics of tilting process.

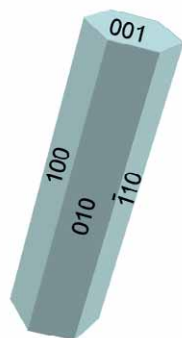


Fig. S5 Schematic diagram of a single CuInS₂ nanorod