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Observation of Dynamic Structural Transformations in a Copper Sulfide Nanorod by TEM

Haimei Zheng[1*], Jessy B. Rivest[2], Tim Miller[3], Bryce Sadtler[1,4], Aaron Lindenberg[3], Lin-Wang Wang[1], Christian Kisielowski[5], A. Paul Alivisatos[1,4]

[1]*Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

[2]*Department of Mechanical Engineering, University of California, Berkeley, CA 94720, USA*

[3]*Department of Materials Science and Engineering, Photon Science, Stanford University, Stanford, CA 94305, USA*

[4]*Department of Chemistry, University of California, Berkeley, CA 94720, USA*

[5]*National Center for Electron Microcopy, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

Copper sulfide has been studied extensively for solar cell applications due to their favorable band structures and the well-matched absorption spectrum with the solar spectrum. There are a number of copper sulfide phases with the Cu:S ratio close to 2:1 and at 376 K copper sulfide transforms from low- to high-chalcocite phase. An understanding of the microscopic mechanisms of structural transformations is critical for controlling the metastability of the material and the long-term performance of the solar cell devices. Critical predictions of phase transition theory are that the system fluctuates between two equilibrium structures near the transition point and that the region of transition broadens in small crystals. Here, we report the direct observation of structural fluctuations within a single copper sulfide nanorod using an aberration-corrected TEM (TEAM0.5). We have observed trajectories of structural transformations in individual nanocrystals with atomic resolution, which reveal an unprecedented level of details on the fluctuation dynamics, including nucleation, phase propagation, and pinning of structure domains by defects. The clear influence of the surface and interface energies on nucleation and pinning phenomena suggest strategies for stabilizing particular metastable structures.