Nanoscopic Structures Transiently Formed at the Phase Boundary During Structural Phase Transitions

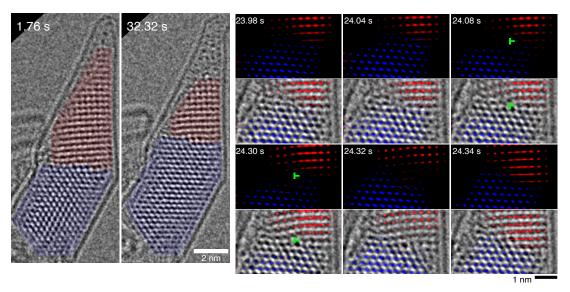
(¹Department of Chemistry, The University of Tokyo)

OMasaya Sakakibara, Takayuki Nakamuro, Eiichi Nakamura

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Structural phase transition, the interconversion between distinct crystal structures, ubiquitously occurs in metals, alloys, and ionic crystals. While a detailed understanding of the process is desired to control material properties, the atomistic mechanism has not yet been fully revealed due to the absence of suitable analytical methods to study nanoscopic local dynamics at the phase boundary. Here we report the direct visualization of the structural phase transition of alkali halide nanocrystals by single-molecule atomic-resolution time-resolved electron microscopy (SMART-EM) technique² and the clarification of the local structural dynamics at the phase boundary during the process.

Through SMART-EM observation of CsCl nanocrystals encapsulated in carbon nanotubes, a B1(NaCl-type, red)-B2(CsCl-type, blue) coexistence was confirmed in an irregularly shaped carbon nanotube (left figure).³ Under the observation, the position of the phase boundary dynamically fluctuated, and the nanoscopic mechanism of the phase transition was analyzed. Previously unrecognized transient disordering at the interface during the transition was clarified (right). Further investigation clarified that the dynamics varied with the compounds' structural characteristics.



1) T. Meiners et al. Nature **2020**, 579, 375. 2) E. Nakamura, Acc. Chem. Res. **2017**, 50, 1281. 3) M. Watanabe et al. Acta Cryst. **1977**, A33, 294.