

Transient Structural Evaluation of Metastable Nanomixture in Phase-segregation Process

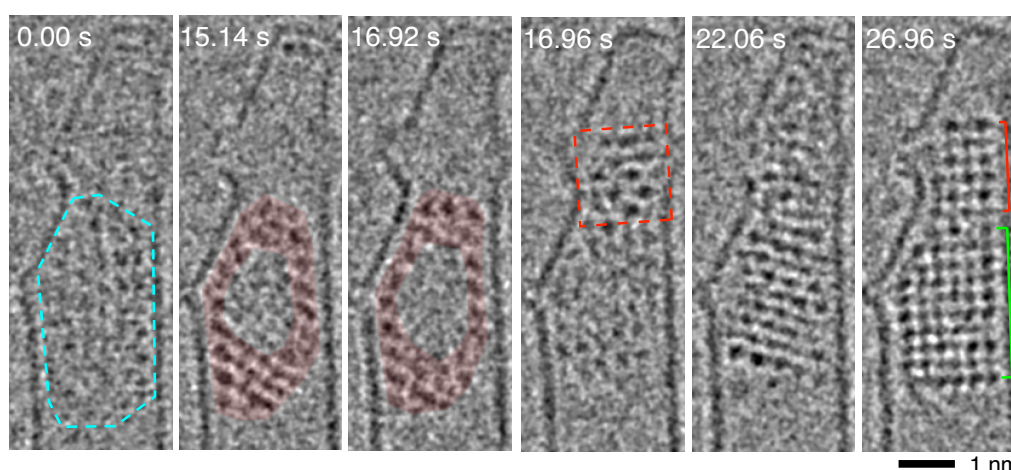
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Phase-segregation plays a crucial role in diverse areas of science and technology including biology or material engineering.¹ Despite its importance, little has been revealed about the atomistic mechanism of phase-segregation due to difficulties in experimental observation of the process with high spatial- and temporal-resolutions. Based on this situation, here we demonstrate in-situ observation of a phase-segregation process on a mixture of sodium chloride (NaCl) and sodium iodide (NaI) inside a carbon nanotube (CNT) by single-molecule atomic-resolution time-resolved electron microscopy (SMART-EM).²

Under SMART-EM observation, a metastable NaCl-NaI mixed cluster without structural periodicity was detected (0.00 s, blue dashed line). After a while, high-contrast local structures were formed on the periphery of the cluster (15.14–16.92 s, red-colored regions), and aggregated at the upper part of the cluster to form NaI nanocrystalline phase (16.96 s, red dashed line). The lower part also transformed into a crystalline structure, forming a NaI-NaCl heterostructured nanocrystal (26.96 s, NaI and NaCl parts were indicated with red and green lines, respectively). The nanocrystals obtained by phase segregation were reasonably matched to their respective bulk crystals. In the presentation, I will discuss detailed analyses of the local structures transiently formed in this process with the aid of persistent homology analysis, a mathematical analytical technique to extract topological features of a dataset.³



1) N. Aihemaiti *et al.*, *J. Phys. Chem. Lett.* **2023**, *14*, 267. 2) T. Nakamuro *et al.*, *J. Am. Chem. Soc.* **2021**, *143*, 1763. 3) Y. Hiraoka *et al.*, *Proc. Natl. Acad. Sci. USA* **2016**, *113*, 7035.