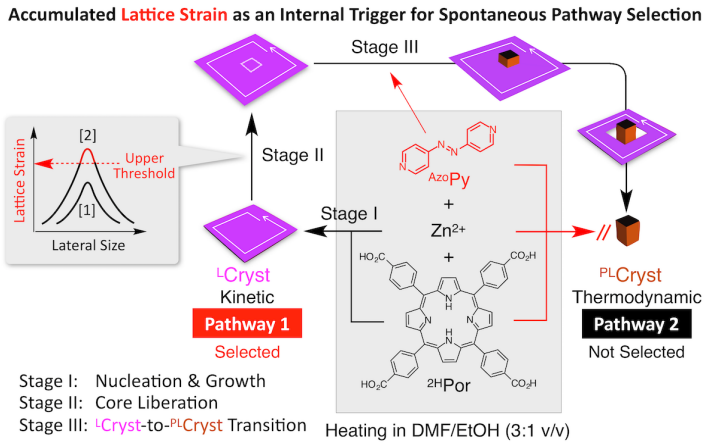
Accumulated Lattice Strain as an Internal Trigger for Spontaneous Pathway Selection

(*Center for Emergent Matter Science (CEMS), Riken*) ○Hubiao Huang

Keywords: Screw Dislocation; Spontaneous Crystal Transition; Lattice Strain; Pathway Selection.

Biological systems are in a far-from-equilibrium state, where a diverse range of components with various lifespans emerge and interact in different pathways before they disappear.[1] Usually, such multiple biological events proceed, in order, because of the timely selection of appropriate pathways. The concept of path-way complexity is highly important, not only in biology but also in other systems including multicomponent assembly and crystallization,[2] and raises the question of how pathway selection can be executed. In a well-designed biological process, a key component that can internally trigger pathway selection may be produced according to a designated timeline.[1] Although a new strategy to mimic biological pathway selection using in-situ produced "internal triggers" has been reported,[3] nonbiological processes have generally been considered to require physical or chemical external triggers for pathway selection.[4]

Here we report an unprecedented finding that a lattice strain accumulated with the growth of a crystal serves as an "internal trigger" for pathway selection in multicomponent crystallization. We discovered a "spontaneous" crystal transition, where the kinetically preferred layered crystal, initially formed by excluding the pillar component, carries a single dislocation at its geometrical center. This crystal "spontaneous-ly" liberates a core region to relieve the accumulated lattice strain around the dislocation. Consequently, the liberated part becomes dy-namic and enables the pillar ligand to invade the crystalline lattice, thereby transforming into a thermodynamically preferred pillared-layer crystal.



Reference: 1. *Nat. Rev. Mol. Cell Biol.* **2008**, *9*, 255; 2. *Science* ***2020***, *368*, 642; 3. *Science* **2015**, *349*, 1075; 4. *Nature* **2012**, *481*, 491.