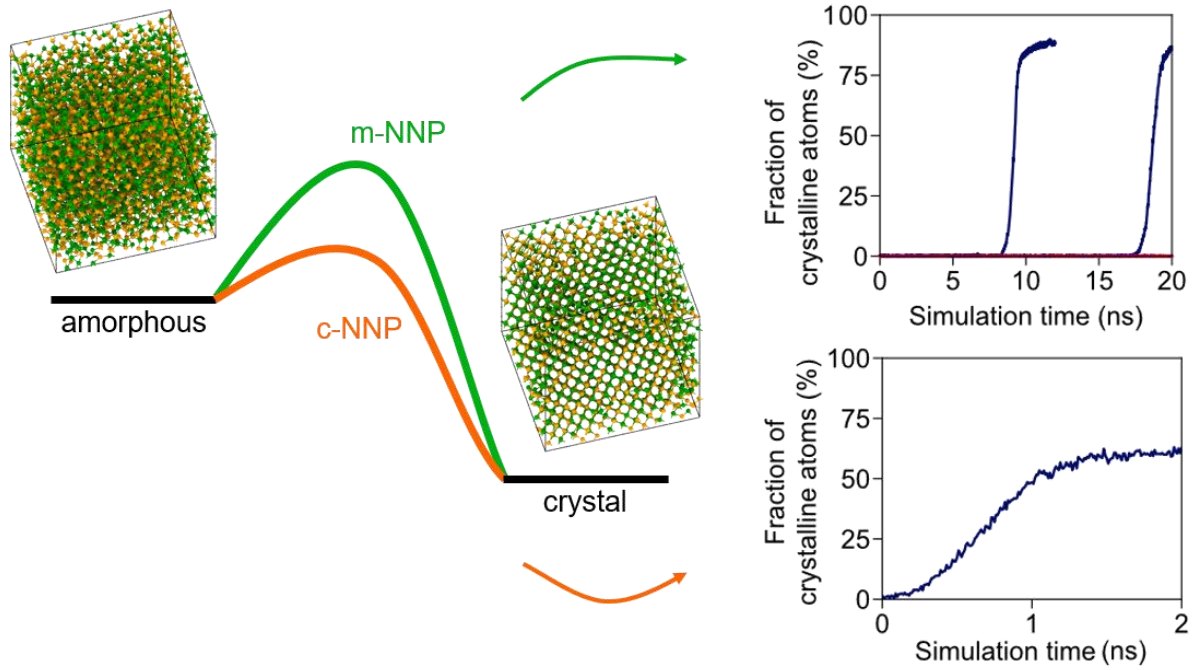
Crystallization of amorphous phase change material



Among various emerging memories, phase change memory has attracted wide interests to compete against conventional memories. In spite of recent commercialization of 3D XPoint by Intel and Micron, slow writing speed (crystallization) is still problematic. Molecular dynamics simulation helps to understand crystallization kinetics in atomic scale. First-principles molecular dynamics gives good insight, but it is difficult to quantitatively compare with experiments due to finite cell. Recently, nueral network potential (NNP) fitted to DFT data enables accurate large-scale crystallization simulation. In this study, we develop reliable NNP for GeTe and simulate crystallization process considering device condition. Nucleation-limited crystallizations are well reproduced,leading to incubation periods of 7 or 17 ns at 500 K. This is in good agreements with the minimum incubation time of 30 ns in experiments. This work was published at Computational Materials Science 2020, 181, 109725.