

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Microscopic pathway of a polymorphic transformation in Al₉₀Sm₁₀ system by molecular dynamics simulations YANG SUN, FENG ZHANG, ZHUO YE, MIKHAIL MENDELEV, RYAN OTT, MATTHEW KRAMER, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory — When as-quenched amorphous Al-10.at%Sm alloy is isochronally heated up, it can display a nearly perfect polymorphic transformation into a complex cubic phase. Knowledge about the pathway of this transformation plays a key role for understanding the phase selection in this system driven far from equilibrium. We successfully simulated the growth of this crystalline phase from the amorphous state using molecular dynamics, with the help of a preexisting crystalline seed. The as-grown structure is in good agreement with experimental X-ray diffraction measurement. By analyzing the atomic trajectories during growth, we show the microscopic pathway linking the amorphous and crystalline phases and how the transformation is controlled by the driving force, atomic diffusivities and structural topologies.

Yang Sun
Iowa State Univ

Date submitted: 14 Nov 2014

Electronic form version 1.4