

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Study the formation of metastable crystalline phases from amorphous metallic systems with an integrated approach ZHUO YE, FENG ZHANG, Ames Laboratory, YANG SUN, University of Science and Technology of China, MIKHAIL MENDELEV, RYAN OTT, EUN-SOO PARK, MATT BESSER, MATT KRAMER, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory — An efficient genetic algorithm (GA) is integrated with experimental diffraction data to solve a metastable $\text{Al}_{20}\text{Sm}_4$ phase that evolves during rapid solidification of an amorphous Al-10%Sm alloy produced by magnetron sputtering. The excellent match between calculated and experimental X-ray diffraction patterns confirms that this new phase appeared in the crystallization of the alloy. We discover the strong similarity of the underlying atomic structure between the amorphous alloy and this phase. Both phases share the same Sm-centered motif, providing a low-barrier pathway to form this $\text{Al}_{20}\text{Sm}_4$ phase in the glass matrix at low temperatures. Molecular dynamic simulations of crystal growth from the liquid phase predict the formation of disordered anti-site defects in the devitrified crystal.

Zhuo Ye
Ames Laboratory

Date submitted: 14 Nov 2014

Electronic form version 1.4