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A genetic algorithm to determine metastable MS1 phase of the Al-Sm system ZHUO YE, FENG ZHANG, YANG SUN, MANH CUONG NGUYEN, MIKHAIL MENDELEV, MATTHEW KRAMER, CAI-ZHUANG WANG, KAI-MING HO, Ames Lab, AMES LAB TEAM — An efficient genetic algorithm (GA) was used to determine a metastable $Al_{60}Sm_{11}$ phase [termed MS1 in Mater. Sci. Eng. A179–A180, 600 (1994)] that evolves during rapid solidification of an amorphous melt-spun Al-10%Sm alloy. The MS1 phase is of particular interest as it is the 1st observed phase during devitrification and is believed to possess a strong connection to the undercooled liquids. It also presents a severe challenge to theoretical crystal structure prediction methods since it 1) has a big unit cell with a $\sim$1.4 nm, 2) is metastable and not necessarily the ground state, and 3) contains site-occupancy and anti-site defects. A GA combined with experimental characterization of phase transitions and Rietveld refinements provides the necessary identification of the MS1 crystal structure. Calculated X-ray diffraction patterns of the MS1 phase match perfectly with experiments. Interestingly, the MS1 phase shares the same motif as undercooled Al-10%Sm liquids. The topological connection between undercooled liquid and crystal structures is worth further investigation, to understand how the topological order in the starting amorphous phase correlates with phase selection during devitrification.

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