Metastable Al-rich phases in the Al-Sm system: A genetic-algorithm study FENG ZHANG, ZHUO YE, Ames Laboratory, IAN MCBREATY, Department of Physics and Astronomy, Iowa State University, MIKHAIL MENDELEV, RYAN OTT, EUN SOO PARK, MATT KRAMER, CAIZHUANG WANG, KAI-MING HO, Ames Laboratory — Metallic glasses formed by Al and about 10% rare earths such as Sm are important high-strength-low-density materials. Various metastable crystalline phases are formed in the early stages of the devitrification of Al90Sm10 glasses. Identification of these phases is crucial to understand the phase selection during amorphization and devitrification processes, and thus provides critical information for the control of microstructures in order to obtain desired mechanical properties. In this study, we use a genetic algorithm to systematically study the low energy Al-rich phases of the Al-Sm system. We discovered a new Al5Sm phase that matches excellently with the experimentally detected M1 phase in lattice parameters as well as diffraction patterns. In addition, we established the energy landscape as a function of Al composition on the Al-rich side of the phase diagram, and found key geometries of Sm-centered local clusters which could serve as building blocks for other metastable phases.

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