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Atom Transport in Random Close Packed Metal Alloys under Thermal Forcing YONG W. KIM, Lehigh University —

Alloy making entails disparate pyro-metallurgical pathways, contributing to variability in elemental composition profiles. Surface segregation by constituent elements is a long-standing example. Thermal cycling and exposures to intense fluxes of energetic particles and photons, as in fission and fusion reactors, force the movement of composition profiles. Transport properties thus become dependent of materials' history. We note that a non-crystalline alloy specimen is a randomly close packed assembly of atoms, and, as such, contains a distribution of residual nano-crystallites. The primary effect of varied forcing mechanisms is to convert atoms bound in nano-crystallites into those of glassy configurations. Spatial fluctuation is increased, specific to elemental species. In this paper we present a modeling of thermal conversion of crystallite atoms into a glassy state. The distribution function of nano-crystallites by size at room temperature is modeled by the distribution of nano-clusters formed from an atomic vapor plume. [Kim, Lee, Belony, Rev. Sci. Instr. **17**, 10F115 (2006)] At a given temperature, equilibrium dissociation of a nano-crystallite into 'glassy' atoms is treated by the law of mass action. The equation of state is fashioned after the thermal expansion of the specimen volume with respect to a reference. A large set of simultaneous dissociation equations is solved iteratively. Work supported in part by NSF-DMR(Metals).

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