Modeling of Thermal Forcing of Non-Crystalline Metallic Alloys

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When non-crystalline alloys are forced thermally into different temperature regimes, the material’s transport properties undergo changes that are dependent of thermal forcing history. (See Y.W. Kim, Int. J. Thermophysics 28, 1037 (2007), and references therein.) Metallurgical processing invariably results in such changes that are frequently non-uniform across the given material specimen. Different structural phases may coexist within such a specimen. If the forcing temperature is oscillated in the course of the processing, the properties may change irreversibly due to restructuring of individual nano-crystallites during cooling. To facilitate first principle-based analysis of a given metallurgical processing, we have embarked on development of a general theoretical modeling framework for temperature dependence of transport properties of binary metallic alloys that are non-crystalline. The theory is built on the thesis that such alloys exist in a randomly close-packed (RCP) state of constituent atoms, and as such, the constituent atoms are distributed in part as nano-crystallites and in another part in a glassy-state of matter. We postulate that when heated, each nano-crystallite undergoes partial thermal dissociation. The heating and the attendant reduction in the sizes of nano-crystallites stimulate atom transport. More mobile atoms tend to accumulate preferentially at the surface due to attraction by their own image charges, leading to development of a non-uniform near-surface profile of elemental composition. Transport properties are computed by Monte-Carlo sampling through the network of nano-crystallites and glassy configurations. The transport of fluxes are evaluated for the sequences of transport in nano-crystallites, in glassy configurations and their transmission across the interfaces between a pair of ordered and disordered media.

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