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 re-structuring 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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