First-Principle Modeling of Disordered Metallic Alloys: Effect of Crystallite Dissociation on Thermal Expansion

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Disordered metallic alloys are modeled as a randomly close-packed distribution of nanocrystallites intermixed with randomly positioned atoms. The crystallite size distribution function is measured in a simulated macroscopic medium in two dimensions. In the system of binary alloys, the distribution function is found to be a stationary random property of the medium for given alloy composition. The degree of crystallinity, which is defined as the probability that a particle in the medium is a member of crystallites, is also determined by the composition. The volume of the macroscopic alloy specimen is then fully defined by the statistical measures. When heated, the nanocrystallites within the specimen become smaller in size as a result of increasing thermal fluctuation. We have modeled this phenomenon as a case of thermal dissociation by means of the law of mass action. The crystallite size distribution function is computed for $AuCu_3$ as a function of temperature by solving some 12000 simultaneous algebraic equations for the degrees of dissociation according to the size distribution of nanocrystallites. The nanocrystallite size distribution function in 3-D is found by transforming the 2-D distribution for this purpose. Linear expansion of the specimen has three contributions: the respective expansions of the crystallites and glassy matter and the temperature dependence of the degree of crystallinity.