

Structure and Energetics of Disordered Materials Using Darwin's Theory of Evolution

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Genetic algorithms have recently found many applications in science. Examples include the prediction of crystal structures and various clusters, studies of protein folding, structure-based drug design, and structure solution from powder-diffraction data. All these applications adopt the principles inherited from Darwinism for finding the best solution to the problem of interest, which involves natural selection of those species which are best adapted to their environmental conditions (selection) and random variations of heritable characteristics (mutation). We show that genetic algorithms and energy minimizations in combination provide a highly efficient tool for mapping low-energy minima on the erratic and complex potential-energy surfaces of grossly disordered materials. The distribution of energy minima mimics with sufficient accuracy the low-energy portion of the parent distribution of minima and allows accurate calculation of configurational Boltzmann averaged structural and thermodynamic properties in cases where a small fraction of the minima is thermally accessible. The distribution of energy minima obtained using genetic algorithms is biased, and consequently the properties converge slowly at high temperatures. In contrast, an optimized set of a few randomly chosen configurations provides a statistical representable selection for the accurate calculation of configurational-averaged properties at high temperatures, but gives a poor description of the low-energy portion of minima. Thus the properties calculated using the random algorithm are hampered by the presence of systematic errors in cases where a small fraction of the minima is thermally accessible. The inherently slow convergence of both the genetic algorithm and the random selection at intermediate temperatures is tackled by combining the lower fraction of the distribution of minima obtained using genetic algorithms with the intermediate and upper fraction from the random (nonbiased) selection of configurations. For this purpose we introduce a cut-and-scale-type scheme. The resulting combined distribution allows accurate calculation of properties at all temperatures.