An efficient Monte Carlo algorithm to study structural relaxation in network forming materials

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Network forming materials are ubiquitous in nature, common examples being semiconductors such as silicon and silica, as well as fluids that can form hydrogen bonds. What these materials have in common is that their topology on short length scales is governed by certain rules.
For example, in amorphous silicon, most atoms are 4-fold coordinated, the preferred Si-Si bond length being ~ 2.35 Angstroms, and the preferred Si-Si-Si bond angle being the tetrahedral angle. This complicates molecular dynamics simulations of these materials, where the particles spend most of their time thermally fluctuating about their equilibrium positions, while large structural changes in the network topology are rare.
To overcome this problem, Wooten, Winer, and Weaire (WWW) introduced a special Monte Carlo move consisting of bond switching Monte Carlo moves which turned out to be very efficient at structurally relaxing networks of amorphous silicon and silica [Phys. Rev. Lett. 54 1392 (1985)]. Unfortunately, the algorithm is only correct when used at zero temperature. In order to also address finite temperature, I propose a modification to the original WWW algorithm such that the Boltzmann distribution is faithfully sampled at any given temperature. The resulting algorithm is used to study the melting transition of a two-dimensional three-fold coordinated network.