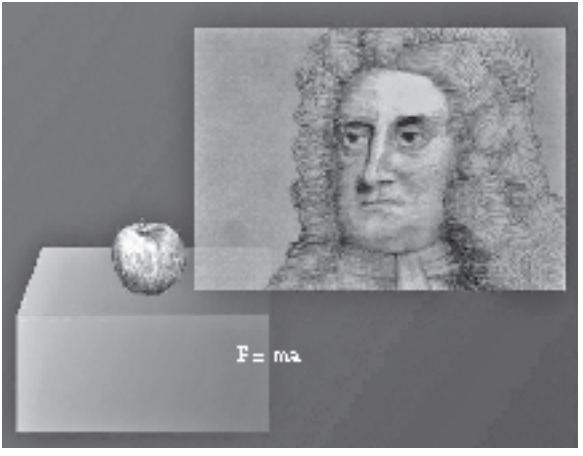

Figure 2.1 Sir Isaac Newton and the apple.

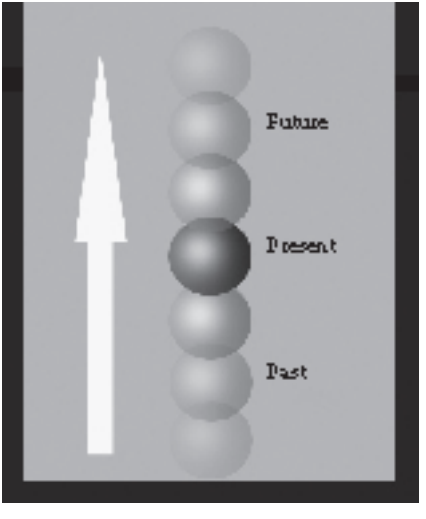

Figure 2.3 A jumping atom (black ball) in a potential well of classical world.

002x003.eps

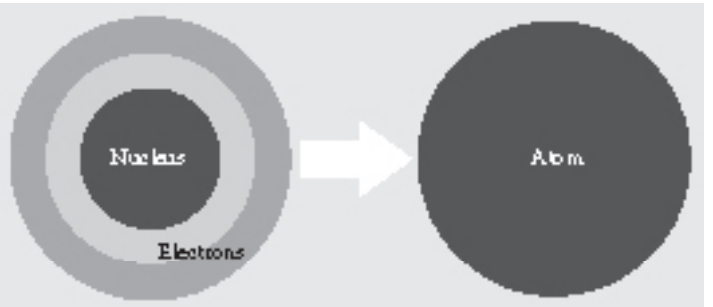

Figure 2.2 Schematic of atomic model in MD methods.

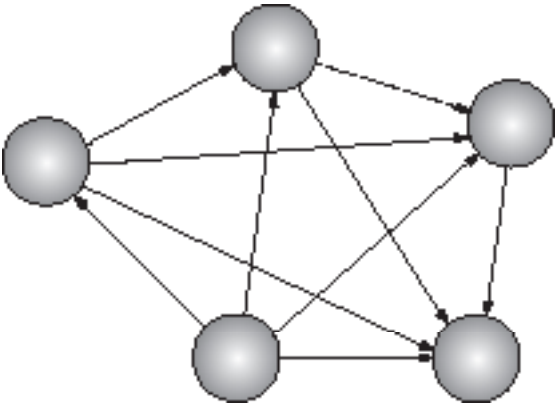

Figure 2.4 Pair interactions (arrows) in a 5-atom system.

002x004.eps

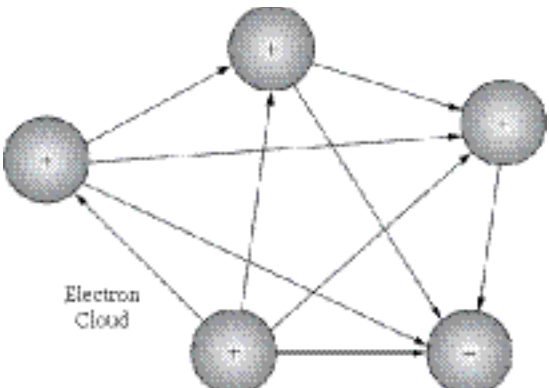

Figure 2.6 Model of 5-atom system for EAM potential showing pair interactions (arrows) and embedding energy (grey area) that represent the *N*-atom effects.

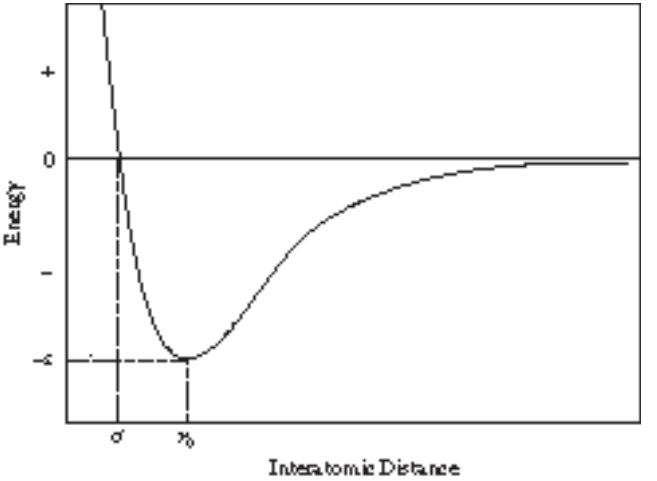

Figure 2.5 Schematic of the Lennard-Jones pair potential.

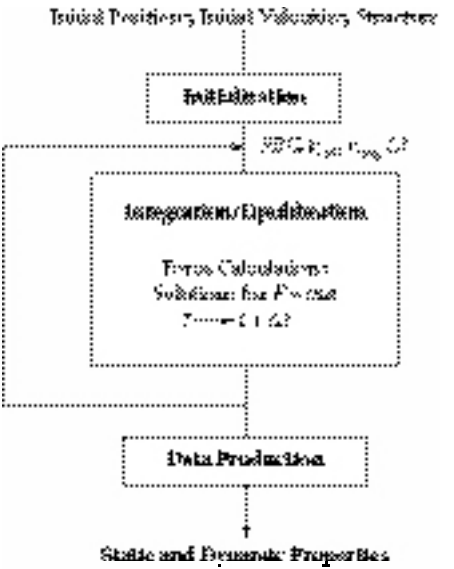

Figure 2.7 Typical flow of an MD run.

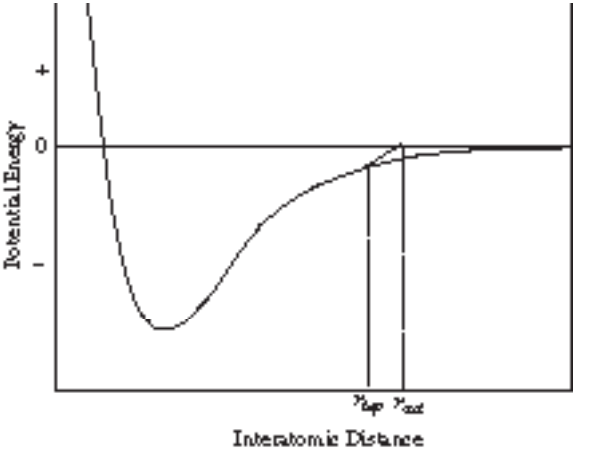

Figure 2.9 Schematic of potential curve with cutoff at r_{cut} and tail-tapering (thicker line) at r_{tap}.

002x009.eps

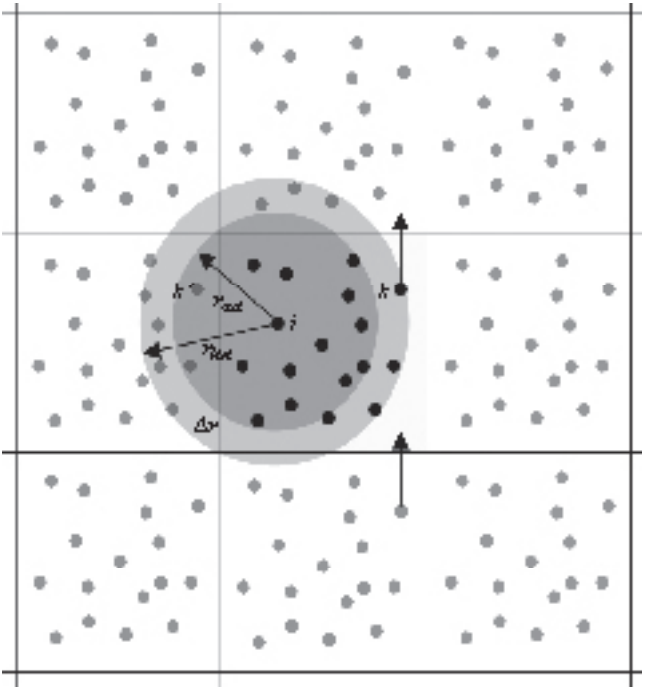

Figure 2.8 Schematic of potential cutoff (small circle) and neighbor-list radius (big circle) under periodic boundary conditions in two dimensions (the primary box at the center and its image boxes around it).

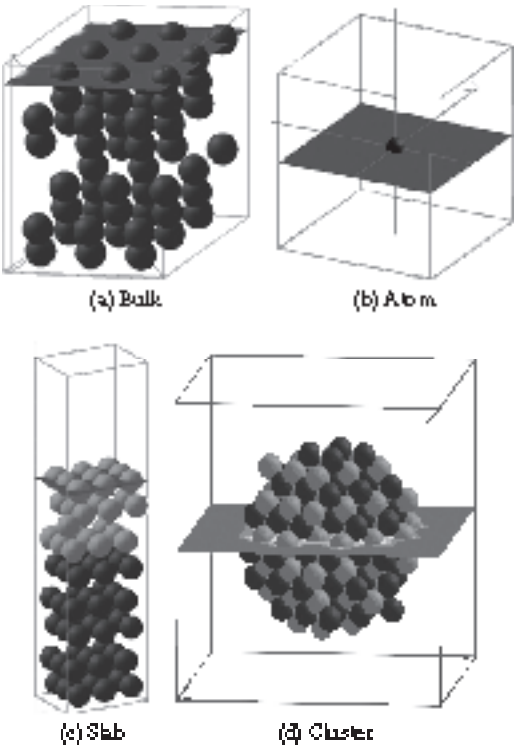

Figure 2.10 Periodic boundary conditions to mimic actual systems with various supercells.

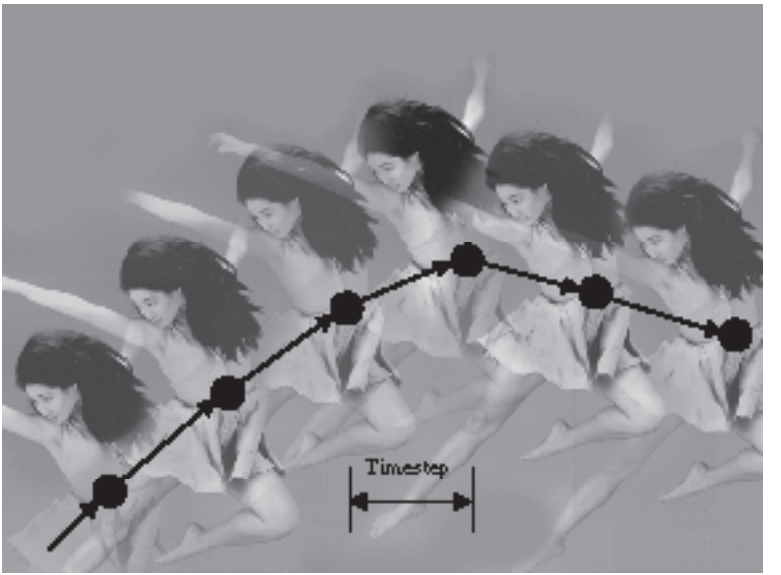

Figure 2.11 Schematic illustration of a trajectory made by a jumping ballerina in five timesteps.

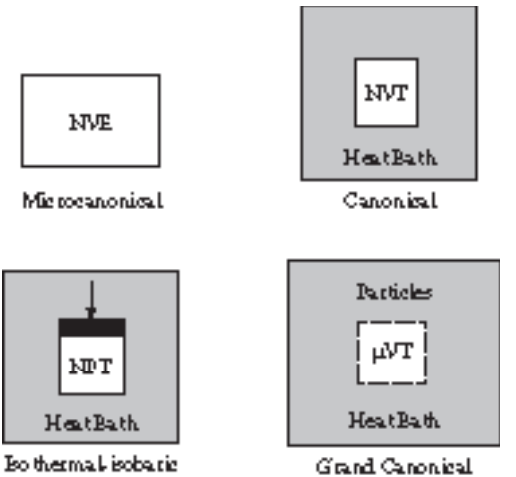

Figure 2.12 Schematics of four ensembles adopted in MD and MC.

002x012.eps

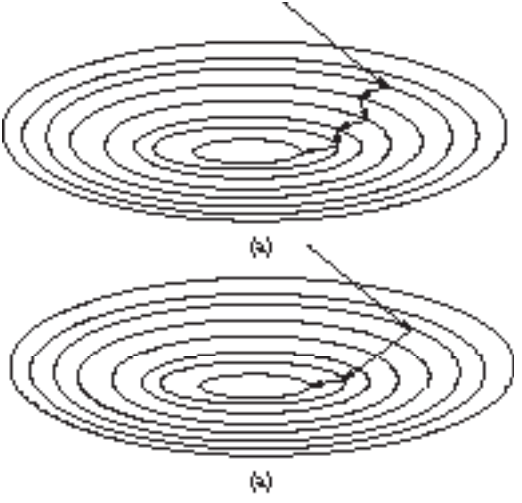

Figure 2.13 Schematics of (a) steepest-descent and (b) conjugate-gradient methods.

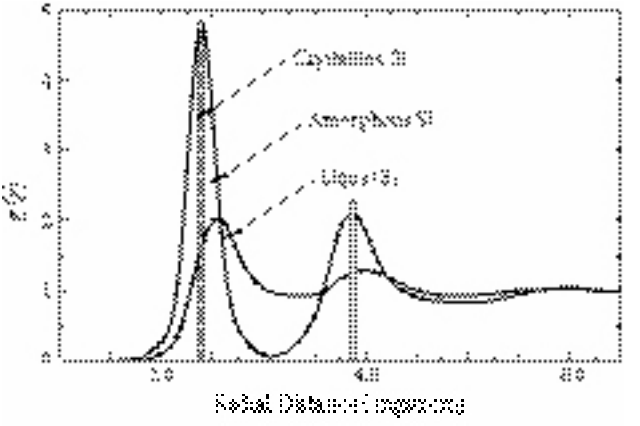

Figure 2.14 Typical radial distribution functions for Si in various forms: amorphous and liquid. (The reference positions for crystalline Si are shown with bars.)