Hybrid Molecular/Cluster Statistical Thermodynamics: A Fast Method to Simulate Quasi-Static Deformation at Finite Temperature

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Abstract: The rapid evolution of nanotechnology appeals for the understanding of global response of nanoscale systems based on atomic interactions, hence necessitates novel, sophisticated, and physically based approaches to bridge the gap between various length and time scales. In this lecture, we propose a group of inter-atomic potential based methods for problems under quasi-static loading at finite temperature, that is, molecular statistical thermodynamics (MST) method, cluster statistical thermodynamics (CST) method, and the hybrid molecular/cluster statistical thermodynamics (HMCST) method. These methods, by treating atoms as oscillators and particles, as well as clusters, comprise different spatial and temporal scales in a unified framework. One appealing feature of these methods is their "seamlessness" or consistency, in which the same underlying atomistic model is used in all regions consisting of atoms and clusters, regardless of additional constitutive relations. On the other hand, compared with conventional MD simulations, their high computational efficiency appears very attractive, as well manifested by the simulations of uniaxial compression and nanoindenation.