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Implementation of isotension ensemble in molecular dynamics

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The implementation of the new type of ensemble, with constant tension force in the molecular dynamic simulations, is considered. In contrast to the isostress NtT ensemble, in which the stress components act on the surface and the volume elements, the new NfT ensemble is determined by the tension forces acting on each particle in the extended space. Correspondingly, instead of the stress-strain relation used in conventional theory, a new type of constitutive equation in terms of stretch and tension becomes an objective of the molecular dynamics simulations. Comparison with the Parrinello-Rahman method is made for the general external load and the temperature applied. Results for the aluminum lattice show that the suggested approach gives an unbiased sampling of the isostress-isothermal ensemble in the LAMMPS environment. Additionally, the problem of atomistic boundary condition was renovated, due to almost identical tension and traction forces. It was shown on several examples of strains that the tension forces properly represent the type and magnitude of the atomistic external load applied to the surface, despite the absence of any quantities related to the area in the constitutive equations. An analog of Cauchy's stress theorem in the new setting is formulated and verified by numerical simulations.

Introduction

A lot of physical processes in the condensed media is accompanied by deformation on the background of thermal motion of atoms. The inclusion of finite deformations in molecular dynamics (MD) requires using additional degrees of freedom. This approximation is based on a strong distinction of the length-time scale, related to the thermal motion of atoms and deformation. Several modifications of the equations of motion have been developed with the usage of additional dynamic variables, such as volume [1] and the MD cell matrix [2]. The isostress approach [2] suggested by Parrinello Raman (PR) is exclusively widespread in MD calculations to study condensed phase systems. In this approach, the simulation cell is allowed to change its shape, appropriately conforming to the external stress tensor. The components of stress, being a continuous field, act over an area. It doesn't look quite natural from the point of MD, whose equations of motion inherently exploit molecular variables. You have to use constraints to scale the coordinates of particles to a flexible MD cell. One inconvenience of such schema follows from a change of instantaneous orientation and size of surface elements while the body deforms. In correspondent Lagrangian framework, instead of true (Cauchy) stress as the external load, the second Piola-Kirchhoff stress is used. As shown in [3], the differences between the two stress measures may be significant in calculations using the PR algorithm. Although this obstacle was overcome recently, a special procedure of adaptive control of stress at each MD step [3] hardly seems quite natural.

In continuum mechanics, a deformation mapping between current and reference configurations is given in terms of quantities belonging to the deformed body. In particular, PR method used the cell vectors for this purpose. The alternative algorithm suggested in [4] involves no values referring to any surfaces or volumes. Correspondent treatment has a rigorous geometric background [1] based on the representation of classical mechanics in $^{6} = {}^{6}$ manifold. Six true topological dimensions of the torus surface are represented by six scalars: three stretches and three shear angles. These scalars specifying the Euclid metric of the surface by means of an extension of the coordinate space become additional dynamic

[1] Note that the procedure of coordinate scaling in PR method is not 100% correct [5].