

Equivalence of Virial Stress to Continuum Cauchy Stress

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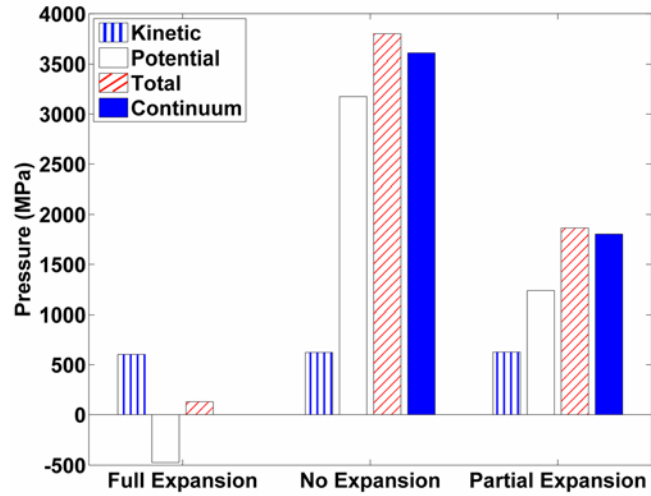
The virial stress derived based on the Virial theorem[1] is defined as

$$\sigma_{ij} = -\frac{1}{V} \left[mv_i v_j + \frac{1}{2} \sum_{q=1}^N (a_p - a_q) F_{pq} \right] \quad (1)$$

where m is the mass of the atom, (i, j) take values of x, y and z (directions), q takes values 1 to N neighbors of atom p , a_p is the position of atom p , F_{pq} is the force on atom p due to atom q and V is the volume.

Calculating stresses in MD simulations is a controversial topic. There are two different schools of thought about the equivalence of the virial stress to the continuum Cauchy stress [2,3]. Zhou[2], based on momentum balance, argues that only the potential contribution (the second term in Equation (1)) to the virial stress should be considered as the continuum Cauchy stress. However, Zimmerman *et al.*[3] assert that the virial stress that contains both the kinetic and potential parts is indeed the quantity that corresponds to the Cauchy stress in continuum mechanics. Here we use a simple thermo-elastic analysis to verify the validity of using the total virial stress as the continuum Cauchy stress.

We considered a 500 atom nickel system with periodic boundaries in all 3 directions. Three separate boundary conditions were used: Free expansion, Partial Expansion and No expansion. Molecular dynamics simulations were performed for all three cases. For the free expansion and no expansion cases, the temperature was ramped smoothly from 0 Kelvin to 500 Kelvin. In the partial expansion simulation, the system was allowed to expand freely (stress free) as temperature was ramped from 0 to 250 Kelvin. Then the boundaries were fixed and the temperature was increased to 500 Kelvin. During free expansion, the Nose-Hoover thermostat and barostat were used to achieve stress free conditions. The figure below shows the results of the simulations. The continuum pressure in the figure is the bulk thermal pressure ($3 \alpha_L K \Delta T$, where K is the bulk modulus, α_L is the linear thermal expansion coefficient). It is clear from the free expansion case that, after the system expands freely, at equilibrium, the potential part of the stress has to be balanced by the kinetic contribution to stress. It is not possible to produce stress free expansion without the kinetic term in the virial stress. Similarly, in the other two cases, the total virial stress is equal to the continuum stress. Hence, it is clear that the total virial stress is the continuum stress.



References

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