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Development of the coarse-grained particle method and its application to compression-wave propagation in metal

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Summary

No limitation exists virtually in target size for the classical simulation of atoms with the O(N) algorithms on parallel machines. On the other hand, the time step cannot be changed and hence the total simulation time still remains short. It is meaningful to increase the time step by the coarse-graining the atomic system. The coarse-grained particle (CGP) method has been proposed for such purposes, but it is applicable only to crystalline solids at zero-temperature limit [1,2]. The total energy of the CGP system is defined as the statistical ensemble average of the atomistic Hamiltonian under some certain constraint. For analytic expression, the harmonic approximation has been used to the inter-atomic interaction, and therefore the finite temperature and anharmonic effects are ignored essentially.

In this talk, we propose a direct Monte Carlo sampling method to calculate the force felt by a CGP at a finite temperature as the finite difference of the free energy. Since we use the inter-atomic interaction potential in its original form, the finite temperature and anharmonic effects are included from the first principles. Significant findings are: (i) The force is proportional to the particle displacement over a wide range. Since the CGP force is some average of the atomic force, the atomic anharmonicity appears to be canceled out. (ii) The force is strongly sensitive not to the temperature but to the volume. The finite temperature effects contribute through the thermal expansion. Therefore we may model to change the quadratic coefficients of the potential function in the CGP system according to the local volume.

Using the pre-computed forces, we construct the potential formula for the dynamics simulation. We perform the propagation simulation of the compression wave in both the CGP and fully atomistic methods for accuracy check.

References

[1] R.E. Rudd and J. Q. Broughton, Phys. Rev. B 58, R589 (1998).

[2] R. Kobayashi, T. Nakamura, and S. Ogata, Mat. Trans. 49, 2541 (2008).