Molecular Dynamics in Submicron Structures Held in Question by Quantum Mechanics

Quantum mechanics negates Molecular Dynamics analysis that assumes atoms in submicron structures have the same thermal heat capacity as in the Bulk.

Sept. 28, 2009 - *PRLog* -- Background
In the 1950s, Metropolis and Teller pioneered molecular dynamics (MD) as a method to derive the thermodynamic and transport properties of bulk molecular liquids. Submicron ensembles comprising a few hundred atoms with periodic boundary conditions were used to derive the bulk liquid properties. Even though the ensembles were submicron, the periodic boundary conditions allowed the heat capacity of the atom at wavelengths longer than the dimensions of the ensemble to be included in the MD simulations.

Today, MD simulations have been extended almost entirely to discrete submicron structures. For example, at the recent World Tribology Council WTC-IV Conference including the satellite on Tribochemistry in Kyoto, the principal focus of research was the local interactions between rubbed surfaces. Discrete submicron structures lack the periodic boundary conditions representative of the bulk, and as such are entities in themselves, e.g., discrete structures comprising a few tens of layers of lubricant atoms between solid walls consisting of a few layers of surface atoms. Other MD simulations included rubbing between a pair of discrete single submicron crystals and the damage to a macroscopic surface from impacting nano clusters of atoms. The implicit assumption in these MD simulations was there is no difference between the thermal heat capacity of the atoms in the discrete submicron structures and those ensembles in MD simulations with periodic boundary conditions used to derive bulk properties in the solid or liquid state.

Problem with MD Simulations of Submicron Structures
Quantum mechanics (QM) as embodied in the Einstein-Hopf relation shows the thermal heat capacity of the atom as given by the Planck energy of the harmonic oscillator depends on dispersion with wavelength. At ambient temperature, most of the thermal heat capacity of the atom is available at wavelengths > 100 microns where the thermal kT energy is about 25,8 meV. However, atoms in submicron structures are confined to thermal emission at wavelengths
Modified MD Solutions
MD simulations of discrete submicron ensembles may proceed as usual provided the QM restriction on the heat capacity of the atoms is properly simulated. Since absorbed EM energy cannot be conserved by an increase in temperature, other means of conservation are required. One such method is the theory of QED induced radiations. See www.nanoqed.org QED stands for quantum electrodynamics. Lacking the heat capacity to conserve absorbed EM energy by an increase in temperature, the absorbed EM energy is frequency up or down-converted by QED to the EM confinement frequency of the submicron structure. Subsequently, the absorbed EM energy is conserved by the emission of non-thermal EM radiation.

To illustrate the QED theory, consider nanoparticles (NPs) that are the common submicron structures ubiquitous to the Earth. Approximated by a sphere of diameter D, the NP is not empty, but a solid having a refractive index n to account for the lower speed of light c/n in the solid state. Upon the absorption of EM energy from the surroundings, QED induces the creation of photons in the NP having Planck energy E = hf, where h is Planck's constant and f is frequency, f = (c/n)/L. Of importance is the EM confinement wavelength L of the NP, L = 2D. However, the QED photons created are only confined briefly because the EM confinement is quasi-bound, and therefore EM radiation of QED photons promptly leaks from the NP, thereby conserving the absorbed EM energy without increasing the temperature of the NP. Depending on the diameter D, the EM energy emitted may be red or blue shift relative to the frequency of the EM energy absorbed. NPs by MD therefore require simulations of atoms by vanishing small kT energy.

Extensions to Typical MD Applications
Extending the QED theory for NPs to the MD simulations of discrete ensembles of atoms depends on the specifics of the application.

1. Rubbing of Tribological Surfaces. MD simulations of rubbing treat friction by the breaking of bonds between the atoms of lubricant and solid surface along the sliding interface. To conserve the bond breaking energies, the lubricant and surface are allowed to increase in temperature. However, atoms under EM confinement are not allowed to increase in temperature. Instead, bond energies may be conserved by non-thermal EM emission into the macroscopic surroundings.

2. Cluster Collisions. The MD simulations of impact of high velocity NPs on macroscopic surfaces correctly allow for temperature increases in the NPs during NP contact. Over the duration of contact, the NP is an extension of the macroscopic surface, and therefore allowed to increase in temperature. However, the instant the NPs rebound from the surface any thermal energy should be promptly conserved by non-thermal EM emission.

3. Rubbing of Crystals. MD simulations of rubbing of submicron crystals showing temperature increases of order 800 K are not valid because non-thermal EM emission conserves rubbing friction without an increase in temperature.

4. Thin Films. Similar to EM confinement across tribological surfaces, heat transfer in thin films from Joule heating proceeds by the emission of non-thermal EM emission. MD simulations showing reduced conductivity across the film thickness are the consequence of the false assumption that atoms under EM confinement have full thermal kT energy. If the MD simulations of heat conduction through thin films over the past 20 years would have been made with atoms at zero kT energy, a temperature gradient would not have been found. This should have raised the flag that conductive heat could only have been conserved by non-thermal EM emission..
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Conclusions
MD simulations that assume atoms in discrete submicron structures have the same heat capacity as those in the bulk are negated by QM. Special attention is required in performing MD simulations of submicron ensembles of atoms that absorb EM energy from the macroscopic environment. Submicron entities cannot conserve absorbed EM energy by an increase in temperature, and instead conservation proceeds by the emission of non-thermal EM emission.

The comments here on MD simulations for atoms under submicron EM confinement are not fatal in that the current MD results may by inspection be readily corrected for the effects of vanishing kT energy and atom heat capacity. MD programs may be revised to include the heat capacity of the atom depending on the EM confinement by tracking the formation of NP clusters during the solution run. Comments of the MD community to the notion of vanishing thermal heat capacity in submicron structures are solicited.

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About QED induced Radiation: Classically, thermal EM radiation conserves heat by an increase in temperature. But at the nanoscale, temperature increases are forbidden by quantum mechanics. QED radiation explains how heat is conserved by the emission of nonthermal EM radiation.

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