DYNAMICAL MEMORY TIME, MOLECULAR RELAXATION CHAOS IN MANY-PARTICLE SYSTEMS

I.V. Morozov, G.E. Norman* and V.V. Stegailov

Institute for High Energy Densities of RAS, Moscow 125412, Russia

Divergence of Molecular Trajectories. Lyapunov instability is inherent to the many-particle dynamic molecular systems. Diverse manifestations of it obtained by molecular dynamics method are given.

Dynamical Memory Time. The concept of dynamical memory time t_m is discussed. The value of t_m determines the time interval during which the behavior of molecular-dynamical system can be predicted from initial conditions and deterministic equations of motion at a certain level of accuracy defined by a particular scheme of numerical integration and time step Δt value. The relation between t_m, fluctuation of total energy ΔE and K-entropy (Lyapunov exponent) is treated.

Chaotic and Dynamic Properties of Molecular Systems. It is concluded that molecular dynamics method is a method which retains Newtonian dynamics only at the times less than t_m and carries out a statistical averaging over initial conditions along the trajectory run.

Homogeneous Nucleation in Metastable States. The simulation peculiarities are treated, which are related to the Lyapunov instability of the molecular systems. The concept of dynamical memory time t_m is exploited. An approach is developed for the estimation of the activation energy and rate for the homogeneous nucleation in superheated solids and liquids. Results for homogeneous nucleation in superheated crystal are discussed.

Boltzmann and Non-Boltzmann Relaxation. Two stages of the relaxation of nonequilibrium two component strongly coupled plasmas were observed. The initial stage is characterized by an oscillatory behavior of kinetic energy of electrons accompanied by a fast relaxation of the velocity distribution function. In the further relatively slow Boltzmann stage the kinetic energies of charges exponentially approach the equilibrium. The character of the relaxation process is compared with the extension of electrons to vacuum from the surface of an initially homogeneous plasma slab.

Conclusion. Meaning of t_m for real systems is related to the thermal and Langevin noise and quantum uncertainty. Possible influence of t_m variation on some characteristics is discussed.

* Phone: (095) 290 1018; Fax: (095) 485 7990; E-mail: *henry_n@orc.ru*