Laboratory of Materials Science for Electronics (2006)

The main objective of our research is to investigate and design novel electronic materials and devices, such as nanostructured semiconductors/ceramics and dielectrics including various plasmas for present and future applications. Large-scale numerical simulations are extensively performed and developments of new algorithms and applications to the numerical simulations are the most important ingredients in our research and education.

Members (2006):
Professor: Hiroo Totsuji (Dr. Sc.)
Associate Professor: Kenji Tsuruta (Dr. Sc.)
Research Associate: Chieko Totsuji (Dr. Sc.)
Students: 2 Doctor course students (including 1 foreign student)
4 Master course students, and 7 Undergraduate students

Subjects:
Structures, dynamics and thermodynamics of charged particle systems;
Coulomb clusters, dusty plasmas and dense metallic hydrogen plasma
Properties of surface and interface of crystals, superlattice, and amorphous semiconductors
Properties of nano-size microclusters of semiconductor

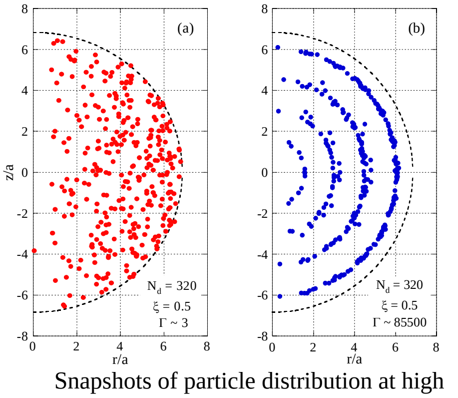
Development of large-scale numerical simulations:
Fast multipole method
Finite element method
Parallel computing using PC clusters
Grid computing

Methods:
Analytical approach
Classical molecular dynamic simulations
Tight-binding molecular dynamic simulations
Density-functional molecular dynamic simulations
Hybrid quantum and classical molecular dynamic simulations

Dust Particles under Microgravity

Ordering of dust particles in dusty plasmas under microgravity,
H. Totsuji, C. Totsuji, T. Ogawa, and K. Tsuruta:
***Physical Review E* , vol.71 (2005) 045401; *ibid.* vol.72 (2005) 036406.**

Structure formation of dust particles in dusty plasmas under microgravity has been simulated by the molecular dynamics method. It is shown that, at low temperatures, dust particles are organized into layered spherical shells. The number of shells is a function of the system size and the strength of screening by ambient plasma particles, while the dependency on the latter is much weaker. In the simulation, the condition of the charge neutrality satisfied by the system of dust particles and plasma particles is properly taken into account.



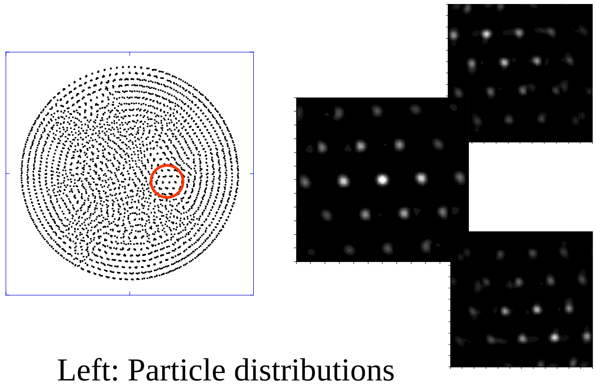
Snapshots of particle distribution at high (a) and low (b) temperatures.

Laboratory of Materials Science for Electronics (2006)

Classical Molecular Dynamics of Many Charged Particles with Fast Multipole Method

Competition between Two Forms of Ordering in Finite Coulomb Clusters,
H. Totsuji, T. Kishimoto, C. Totsuji, and K. Tsuruta:
***Physical Review Letters*, vol.88 (2002) 125002.**

The lowest-energy state of spherical clusters composed of charged particles in a three-dimensional confining potential is investigated. The shell structure in the interior is the lowest-energy configuration for ion numbers smaller than about 10^4, while for larger ion numbers, an interior with bcc ordering surrounded by a few shells on the periphery has lower energy. The formation of a small bcc lattice (nucleation) in the shell-structured cluster is observed.

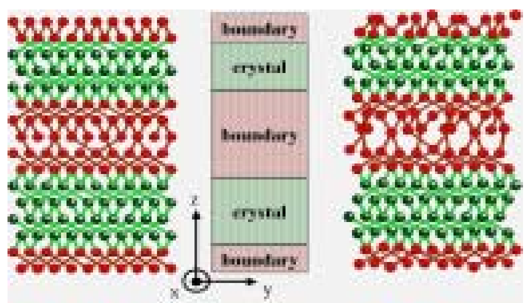


Left: Particle distributions
Right: Observation of Bragg patterns

Tight-Binding Molecular Dynamics on Carbon Crystal with Grain Boundaries

Atomic Structure of Grain Boundaries in Diamond: A Tight-Binding Molecular Dynamics Study,
T. Furubayashi, C. Totsuji, K. Tsuruta, and H. Totsuji:
***Transactions of the Materials Research Society of Japan*, vol.27, no.2, pp.305-308 (2002).**

Diamond is one of the most important materials for electronic applications under extreme conditions (high temperatures, high pressures, etc.). The purpose of this work is to clarify atomic and electronic structures of diamond grain boundaries and their vicinity using the tight-binding molecular dynamics (TBMD) method.



Grid Computing (Collaborations with outside of the University)

Collaborative Simulation Grid: Multiscale Quantum-Mechanical/Classical Atomistic Simulations on Distributed PC Clusters in the US and Japan,
H. Kikuchi, R. K. Kalia, A. Nakano, P. Vashishta, H. Iyetomi, S. Ogata, T. Kouno, F. Shimojo, K. Tsuruta, S. Saini: ***SuperComputing 2002 -High Performance Networking and Computing-*, Baltimore, MD. U.S.A., November 16-22, 2002.**

A collaborative simulation to study environmental effects of water molecules on fractures in silicon has been performed on a grid of geographically distributed PC clusters in the United States and Japan connected over the Pacific Ocean.