

物性研究

「古典粒子系シミュレーションの未踏領域への挑戦」

標題 : Structural and Dynamical Transition in Functional Materials

日時 : 2017 年 6 月 21 日(水) 午後 4 時~午後 5 時

場所 : 柏図書館メディアホール

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要旨 :

Phase transition in condensed matter is an interesting phenomenon from both experimental and theoretical point of view. It can occur either on application of temperature, pressure or field. There exists variety of nomenclature to delineate various kinds of transitional behavior, particularly regarding order of a transition etc. Phase transition has been studied by using macroscopic and microscopic probes. Dynamical transition, viz, order-disorder, sublattice melting, etc. is related to motion of atoms and molecules, leads to many applications. In this context, diffusion or reorientation of a molecular species is of interest in various functional materials. Diffusion is actually a stochastic process. Such a process over a time scale ca 10^{-10} - 10^{-13} sec is conveniently studied using neutron scattering technique. It is particularly suited for studying the dynamics in hydrogenous materials (viz. organic, polymer, soft matter and biological systems etc.) as hydrogen has large scattering cross section. It offers unique possibility of analyzing spatial dimensions of atomic or molecular processes in their development over time. The time-scale of the dynamical motion, its geometry as well as the nature of the hindering potential can be obtained from the neutron scattering data. Molecular dynamics simulation studies are very useful for further insight in the underlying processes as it does not suffer limitations of an experimental setup.

We have studied various systems, for examples, atomic or molecular diffusion (translation and rotation) in crystalline systems, confinement of molecules in nano pores, like clay, zeolites, molecular sieves, metal organic framework etc; polymer based membranes, molecular magnets; nano-metal clusters; micelles and vesicles (a model biological systems) etc. Some of the recent results as obtained from neutron scattering experiments and molecular dynamics (MD) simulation will be discussed.