

AI& Deep Learning for New Material Research



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Keywords Materials science, Iron system materials, molecular dynamics method, diffusion coefficient, information processing materials, amorphous materials, relaxation phenomena

Technical Support Skills

- Measurement of the diffusion coefficient of atoms
- Numerical processing in Python and deep learning
- Fundamentals and applications of materials related to phonon and magnetism

Research Contents New Material Development and Visualized Atomic Diffusion Studies Using IoT Deep Learning

IoT Deep Learning for New Material Development
3D AVS Player Research on numerical processing for automated video visualization,
especially visualization of atomic diffusion in Iron-based materials by molecular dynamics method

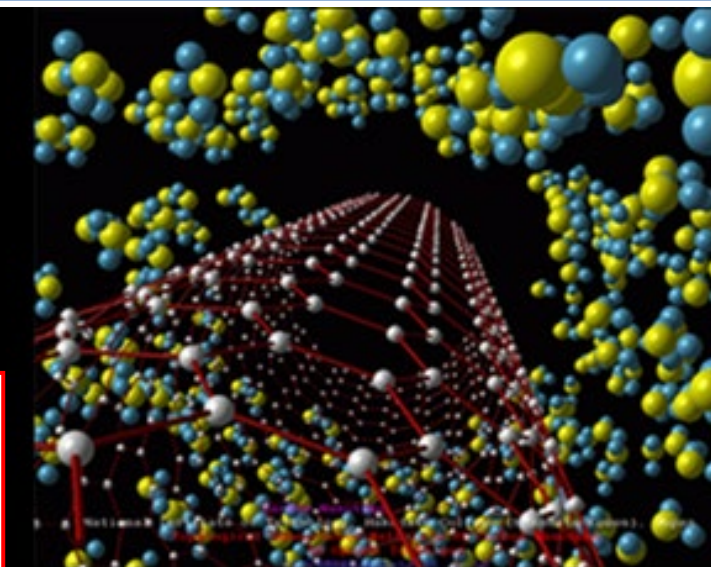
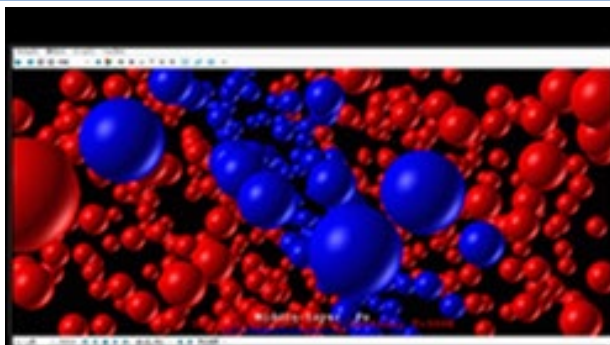
The focus is on information processing of materials science. The convenient 3D AVS Player can play back 4D animations of AVS/Express and MicroAVS visualization results (viewpoint can be changed during playback), and is being deployed in new materials development using IoT deep learning.

The 3D AVS Player is currently available in Japanese, English, and Chinese, and is distributed free of charge in MS-Windows 32-bit and 64-bit versions.

In this study, we apply Python open source libraries to deep learning for new material development, especially for visualization of atomic diffusion in iron-based materials by molecular dynamics. The data used are not limited to mechanics; a wide variety of data can be used. In addition, we will especially focus on the greatest advantage of molecular dynamics, which is the ability to numerically explore the diffusion coefficient of atoms by the only means available, and apply the results, both quantitatively and qualitatively, especially to atomic diffusion in iron-based materials, to develop new functions for materials closely related to both optical and magnetic aspects, such as high-density magnetic recording materials.

The application of visualization techniques to the structural results of the above materials provides a broader perspective to the discussion of the thermal stability of materials.

The following (left) is a time-tracking and visualization of thermal diffusion of atoms in a multilayer in an iron-based material, which may lead to new structural and magnetic materials. The following (right) is a time-tracking and visualization of hydration in a carbon-based material, which is expected to be used, for example, for the application of a mechanism to efficiently transport drugs into the body.



Left: An example of Fe multilayer in a 4D movie in which all atomic positions are calculated from the computer and the viewpoint can be changed flexibly. Right: A time-dependent hydration in a carbon-based graphene material is visualized and applied, for example, to a mechanism for efficient drug delivery into the body.

Available Facilities and Equipment

Scientific Plot PDF Creation Software Operating Env.	3D Scientific Diagram Python Operating Environments
4D Movie Automatic Generation Operating Environments	Differential Scanning Material Property, Calorimetry
GMR, Giant type Magneto-Resistance Sensors	Hall-type Giant type Magneto-flow Sensors
Real-time Facial Surface Geometry from Video on GPUs	Real-time Facial Surface Geometry from Monocular Camera
Real-t-Hand/Body Geometry from Monocular Video GPUs	Real-time music acoustic spectrum analyzer from on GPUs