Finemechanics

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Department of Finemechanics

Soyama/Sasaki Laboratory


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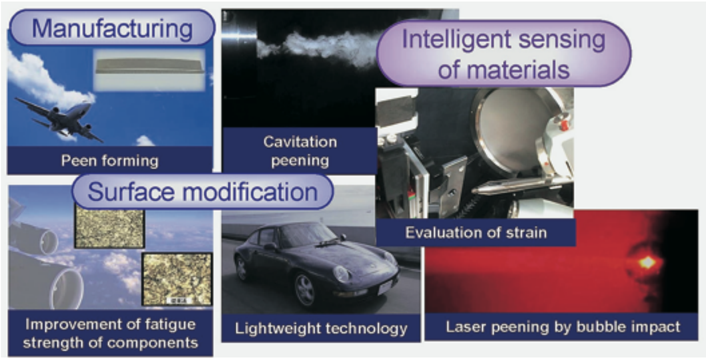
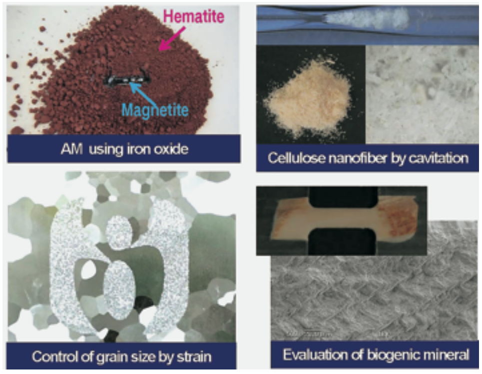
Materails Physics and Engineering,
Intelligent Sensing of Materials

http://www.mm.mech.tohoku.ac.jp/menu4/peening/shotless.html



Surface mechanics design based on mechanical surface treatment and evaluation of materials



Generation of novel materials

Surface mechanics design for improvement of reliability of components

In order to establish sustainable society, surface mechanics design by using surface modification, which is developed in our lab, has been applied to improve reliability of components such as enhancement of fatigue strength. As the surfaces of components are exposed to severe condition in view point of mechanical and chemical conditions, the reliability of components can be improved by surface mechanics design. In our lab., mechanical surface treatment using cavitation impacts which normally cause severe damage in hydraulic machines has been developed in collaboration with a worldwide major company of aeronautical industry, it is called as cavitation peening.

Additive manufacturing of iron oxide by using CW laser

In order to realize additive manufacturing on Mars and/or Moon, additive manufacturing of iron has been investigated in our Lab in collaboration with Johnson Space Center, NASA. In our experimental research, we can make a component from iron oxide using a continuous wave laser. We proofed that oxygen was obtained during the process. Namely, we can get the component and oxygen at the same time. And also we are investigating the strength of the components using our inverse method.

Improvement of Fatigue Strength of Biomedical Implants

In order to apply biomedical implants safety, the improvement of fatigue and fretting fatigue strength are required for the biomedical implants such as rods for the spinal implants. In our lab., the mechanical surface treatment to enhance fretting fatigue strength of biomedical implants has been developed in international collaboration research projects.

Cellulose nanofiber CNF by using hydrodynamic cavitation

Cellulose nanofiber CNF is an attractive material in view point of sustainable and ecological material. However, the production of CNF from naturally-derived cellulose is still very difficult. In our lab., the method using hydraulic cavitation has been developed to produce CNF.

Novel material considering biomineralization

Biogenic mineral produced by biomineralization is attractive material as it is lightweight and high toughness. In our Lab., additive manufacturing of calcium carbonate considering biomineralization has been developed using a continuous wave laser. The mechanical properties of additive manufactured calcium carbonate and biogenic mineral such as shell are evaluated by using inverse analysis.

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Aoyagi Laboratory

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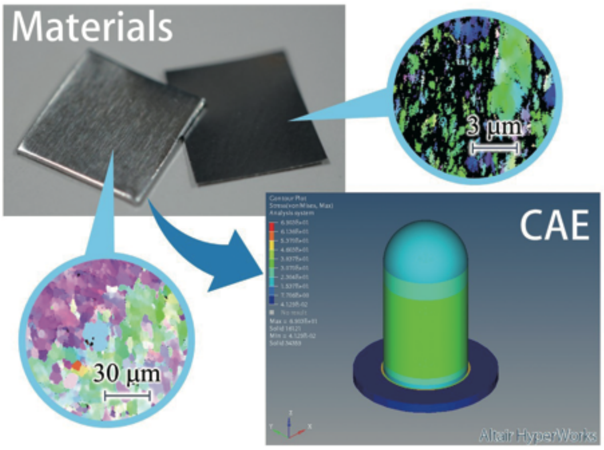
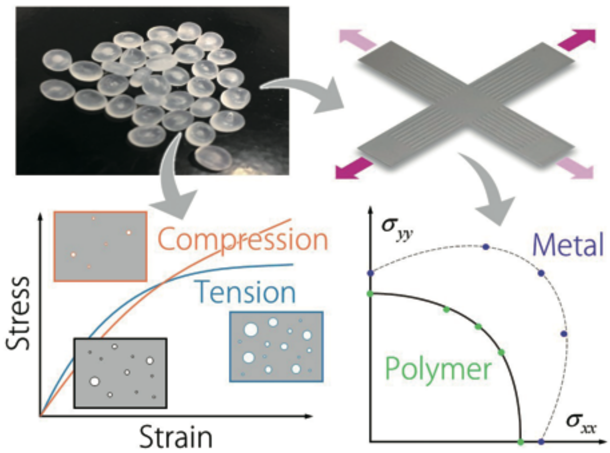


Prediction of Mechanical Properties Based on Microstructures of UFGMs



Evaluation of Mechanical Asymmetry and Anisotropy for Thermoplastic Polymers

Multilateral Plasticity on Advanced Materials

Metallic and polymeric materials, which are indispensable for our daily life, are developed for application under severe environment and weight reduction of structures. To enhance formability and reliability of the advanced materials, we are expecting the construction of theoretical models that can understand the mechanical properties based on the microscopic behavior of the material and express the deformation behavior of the advanced material. In this laboratory, complicated behavior of materials is calculated using MULTILATERAL PLASTICITY. Furthermore, we aim to unite the data obtained by experiment with computational research and to create new prediction.

Simulation on Mechanical Properties of UFGMs

It is well known that mechanical properties of metals improve as grain size decreases. However, the microscopic mechanism of “Ultrafine-Grained Metals: UFGMs” whose grain size is less than 1 micron is unclear. In this study, FEM analysis considering a role of grain boundary as dislocation sources is carried out on Al polycrystals with different grain size, and change of yielding behavior with decrease of grain size is investigated.

Polymer Plasticity Based on Microscopic Structures

The crystalline polymer material consists of an amorphous phase with random coil structure and a crystalline phase in which molecular chains are regularly arranged. Although industrial demand is strong for research on such materials, the characteristics of each phase are unclear. In this study, we construct a new polymer plasticity model with mixed crystalline and amorphous parts based on experimental observations on the deformation behavior of spherulites.

Creation of CAE System Predicting Mechanical Properties

We numerically predict yield function used for CAE of structure analysis. We use the experimental multiscale plasticity model describing deformation behavior based on information on the microscopic structure of materials obtained from experiment observation and measurement. We aim to seamlessly connect a series of CAE processes (material design, development, and practical application) by introducing the obtained yield function into general structural analysis software.

Effect of Trancecrystal on Mechanical Properties of FRTP

The properties of fiber reinforced thermoplastic (FRTP) composites are affected by crystal structure called transcrystals around reinforcing materials and the size of spherulites. In this study, we produce a thermoplastic composite with different crystal structure of the base polymer by changing thermal condition at molding. Then, we evaluate the effect of crystal structure on thermoplastic composites by measuring the mechanical properties.

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Unique products developed by industry-university cooperation

New Industry-Academia-Government Collaboration, Sendai-Hokkirigwa Model

We have been continuously disseminating unique findings and products, such as novel materials and advanced mechanical systems, from Sendai to the world. The new style of Industry-Academia-Government collaboration have been well known as Sendai-Hokkirigwa Model. The target fields are industry, medical welfare, life support, sports, and so on. Due to the achievement, we were awarded a lot of prizes by the Cabinet and government agencies. In addition, we have had many opportunities for technical support to more than 1,600 companies and made a contribution to society.

Low-friction and low-wear materials

We have been developing composite materials filled with RB ceramics particles as low-friction and low-wear filler. A dry-type stainless chain was put to actual use using the RB ceramics composite. A metal/RB ceramics composite, which was developed as a slider of railway collectors, exhibits much higher wear resistance than the conventional slider material. We expect that the material will be use in actual trains.

High-friction and low-wear materials

We have been developing high-friction materials to a wet surface using RB ceramics particles. The high-friction materials are applied to a high-grip rubber shoes, a high-grip tires for sports-specific bicycles, a self-propelled nondestructive inspection instrument for electricity distribution lines. On the other hand, high-slip-resistant kitchen shoe, of which surface patterns were optimized to obtain high friction on a wet flooring, have had attractive attention through mass media.

High-functional tapping tool

From the Industry-Academia collaboration, we have developed tapping tool covered with nickel/abrasive particles composite film for preventing chip snarling. The tapping tool can prevent the chip snarling at high machining speed (five times as high as the conventional process). This will contribute to reduce the process time and process cost.

Facial tissue paper with excellent textural properties

From the Industry-Academia collaboration, we found parameters to evaluate the textural characteristics of facial tissue paper, which was "frictional index to skin". Using the findings, improvement of paper quality was achieved without higher manufacturing costs and the facial tissue paper have been a commercial reality with excellent textural characteristics.

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Yamaguchi Laboratory

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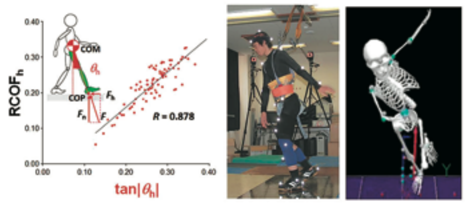
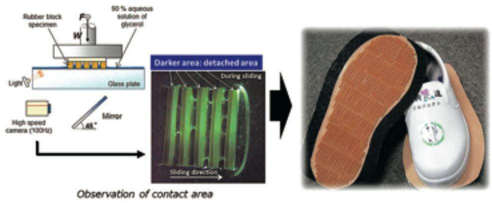
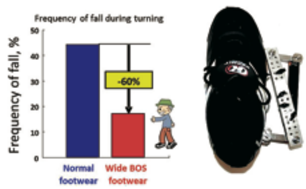


Mechanism of slip-related fall during walking



Development and application of high friction rubber



Development of shoes for fall-prevention

Friction testing apparatus

Development of low friction and low wear polymer composites

Life Support Tribology for Safe and Secure Society

Our laboratory aims to perform the following researches in order to prevent falling accidents due to induced slip during walking.

1) Mechanism of slip-related falls based on kinetic and kinematic analysis of gait
2) Investigation of friction coefficient needed to prevent slip between shoe sole and floor/road surfaces
3) Proposal of gait with low slip risk
4) Development of high grip sport shoes

We have succeeded in development and commercializaion of safety sandals for hospital patients, super high slip resistant rubber sole of working shoes, high slip resistant concrete block for walkway by industry-academia collaboration.

Development and application of low friction and low wear polymer composite

Usage of polymer materials have been expanded in mechanical system as alternative of metalic materials. We have developed polymer composite materials filled with hard porous carbon particulate made from rice bran. The composite materials exhibite low friction and low wear compared with polymer compoistes using conventional fillers. We apply this new polymer composite materials to mechanical systems such as dry stainless chain, guide vane bearing of hydroelectric generator.

Development and application of high friction and low wear elastomer

Rubbrer materials used in automobile tire and sole of sport shoes require high friction on wet road surfaces. We have studied material design and shape of rubber tread blocks for high friction under wet conditions as well as imporovement of wear resistance. We have succeeded in the developement of super high friction rubber sole pattern which enables ascending 40 degrees ramp wet with oill.

Development of tribo-testing apparatus

We have developed the following friction tester:

1) Friction tester which enables collecting friction and wear data under a varied normal load conditions at a single sliding test.
2) Friction tester which enables collecting friction coefficeint under a wide sliding velocity conditions at a single sliding test.
3) Portable shoe-floor friction tester which enables collecting static and dynamic friction coefficient at shoe-floor interface under normal load and sliding velocity conditoins close to those during human locomotion.

Industry-academia collaboration and education

Our laboratory tries to return the research results to society by industry-academia collaboration. We are doing research and education together with Hokkirigawa-Shibata lab. For more detail, please see our web site.

Finemechanics
Fracture and Reliability Research Institute

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Strength and Reliability of Nano- and Micro-scale Materials and Structures

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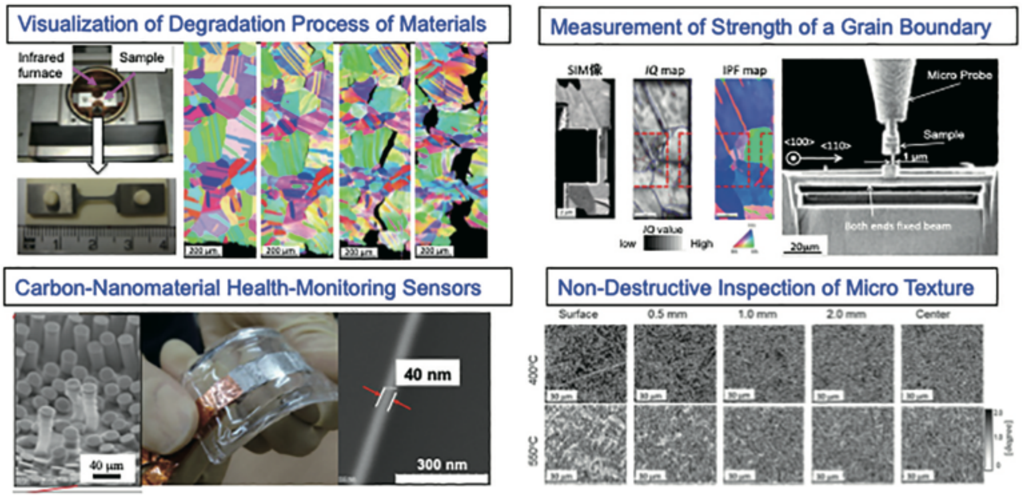

Prediction and Prevention of Fracture of Advanced Materials

Degradation of materials has been accelerated in various social systems used under harsh conditions such as high temperature, high speed, and large capacity. In order to prevent any failures and fractures of materials and devices, it is indispensable for developing the quantitative evaluation method. The main researches in our laboratory are the development of 1) visualization method of micro texture of solid materials in an atomic scale, 2) Design and fabrication method of functional materials, 3) health monitoring method of industrial structures, and 4) non-destructive inspection method of materials damage.

Visualization of Atomic-Scale Degradation of Materials

The change in the alignment of atomic configuration in materials under operation is visualized by using electron back-scatter diffraction. The change is dominated by the stress-induced anisotropic acceleration of atomic diffusion of component elements. The activation energy of atomic diffusion is drastically decreased by tensile stress, and thus, local composition and atomic configuration are shifted aisotopically.

Design and Fabrication of Advanced Functional Materials

Highly reliable material are designed by using atomic scale simulation, considering the suppression of the stress-induced migration of atoms. The main issue is the development of the controlling method of the quality of grain boundaries and atomic doffusion around the grain boundaries. In addtion, the designed materials are produced experimentally and their performance and reliability are evaluated quatitatively.

Health-Monitoring Sensors and Technologies

Various sensors are developed for monitoring the operating conditions of structures and materials. Carbon nanomaterials such as carbon nanotube and graphene nanoribbon are applied to the sensors by using their strain sensitivity of resistivity, activation energy of chemical reactions and so on. Highly reliable and sensitive sensors are developed for our safe and reliable society.

Non-Destructive Inspection of Damage of Materials

The change of micro texture of various materials is observed by detecting the change in their local surface reflectance by using high-resolution spectrometer. The changes of not only the local distribution of elements, but also the local plastic deformation are observed by detecting the change in the spectrum of the reflected light. In addition, micro tensile test system is developed for maesuring the change in the strength of a garin and a grain boundary in various materials.

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Design and Evaluation of Function and Reliability of Materials
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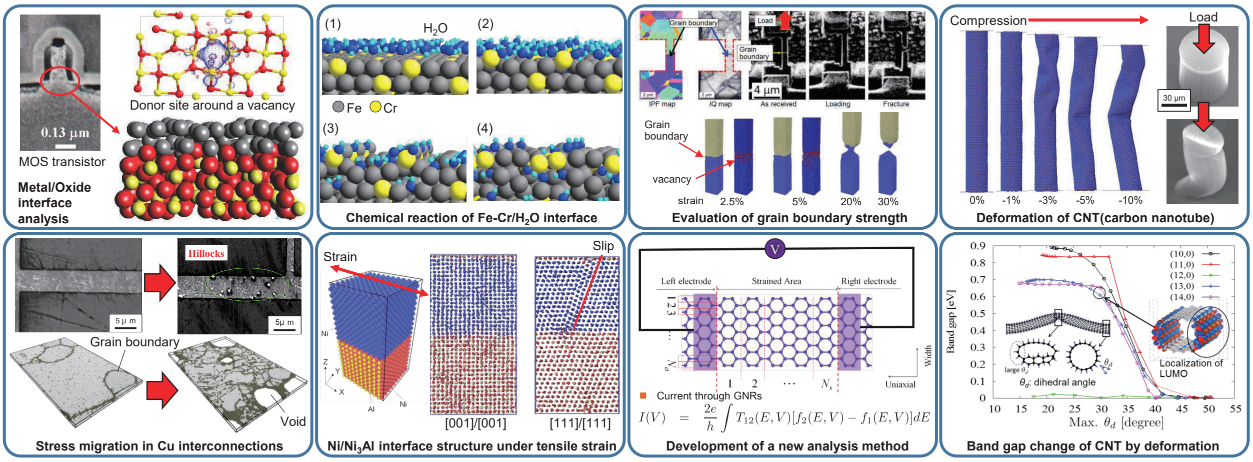

Explicating the fluctuation mechanism and design of the functional interface integrity based on atomic-scale simulations

Design of Interface Integrity Based on Atomic-Scale Simulation

Advanced material systems consisting of multi element, phase and micro texture have heterogeneous interfaces inside materials. The heterogeneous interface structure and its associated physical-chemical properties often change with time due to the gradients of composition, temperature, strain, and so on, which degrades the performance and function of the material system under operation. From this point of view, in order to design the interface integrity for ensuring the reliability of material systems, dominant factors cause the change in the interface structure under stress or strain are determined by using computational simulations and experimental methods.

Atomic-Scale Simulation Based Material Design

The mechanism of the change in heterogeneous interface structures between stacked thin-films, precipitate/matrix interface and metal/environment interface has been studied by focusing on the strain-induced and accelerated atomic diffusion. To improve the performance and reliability of macro and nano-scale products, we have been developing methods for optimizing the interface structure, material, and fabrication process by the combination of atomic-scale simulation and experiments.

Development of Analytical Methods

We have been developing analytical methods based on electronic- and atomic-level computational simulation techniques such as tight-binding based Green's function method for explicating fluctuation mechanisms of the interface structure and physical properties caused by atomic-scale damage and defects. In order to validate the analytical results and improve the simulation accuracy, the change in physical properties are measured by using micro- and nano-scale measurement methods.

Degradation Mechanism Analysis of Heat-Resistant Alloys

In order to clarify the degradation mechanism of heat-resistant alloys such as stainless steel and nickel base superalloy under high temperature creep, fatigue and creep-fatigue conditions, the fluctuation mechanisms of their functions such as strength and corrosion resistance depending on micro and nano texture: composition, defects, impurities, crystallographic orientation, interface and grain boundary structures have been investigated by using the computational chemistry approach.

Electronic Structure Analysis of Carbon Nano Materials

Carbon nano materials such as graphene and carbon nano tubes have high electron mobility, high mechanical strength and large deformability. By utilizing these superior properties, we have been developing carbon nano material based sensors such as strain sensor, tactile sensor, gas sensor and photodetector. For improving their performance and reliability, strain and structural dependence of the electronic band structure of carbon nano materials has been investigated.

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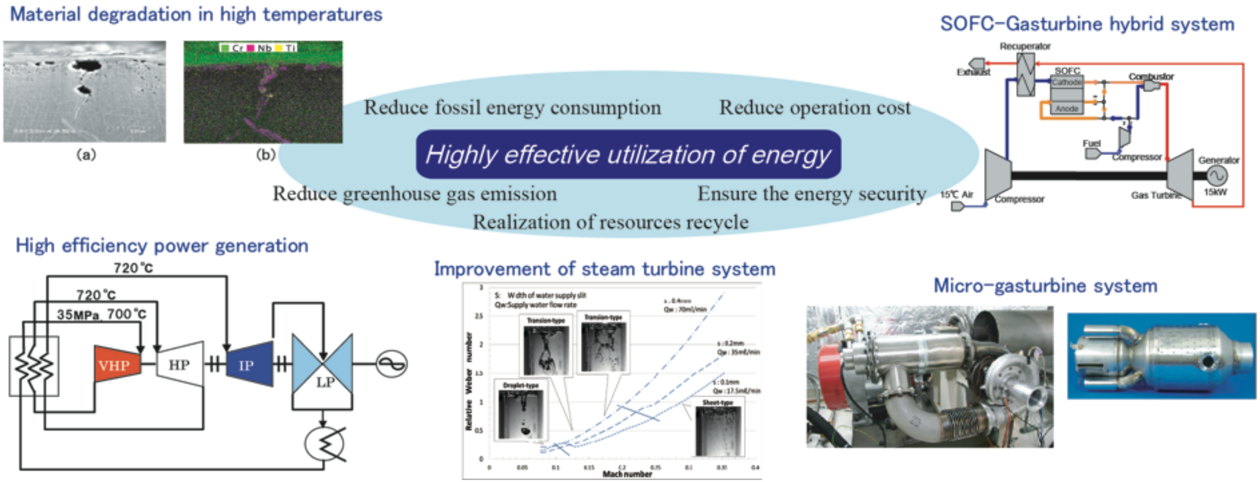

Establishment of Advanced Energy System for Efficient Use of Energy

The objectives of researches are to investigate the issues related to the improvement of efficiency and serviceability of fossil and nuclear power plants, and subjects on the sophistication of maintenance. With aiming to establish the sustainable operation of the electric power plants, the material degradation behavior in the high temperature steam environment and the droplet formation behavior around the steam turbine blade are experimentally investigated. We are also developing a new system with a function to absorb excessive power using a turbine system, aiming to develop a highly efficient and reliable system in harmony with renewable energy.

Characterization of Heat Resistant Alloys for Power Plant

Coal is expected to provide a stable supply, and pulverized coal power will continue to be a part of the power source. The advanced ultra-supercritical (A-USC) power plant is being developed to increase the efficiency in order to effectively use resources. With focusing on the change in material properties during long term operation, effects of steam oxidation and precipitations induced from the fabrication and/or welding process on cracking paths of alloys for A-USC are evaluated.

Performance Characteristic Analysis by Dynamic Simulator

Research purpose is to develop dynamic simulators for advanced electric power generation systems which have not only high efficiencies to decrease exhaust carbon dioxide, but also functions for load following with absorption of the excessive power generated by renewable energy to keep stable power grid. The feasibility of the systems, optimization of the system, solutions for several problems which will be encountered in real machines, are studied by using the dynamic simulator.

Mechanism and Reducing of Damage in Wet Environments

In a steam turbine system, when a droplet in a cascade hits a subsequent blade, a braking effect occurs, causing a reduction in efficiency and material damage. For the low pressure steam turbine, studies on the behavior of water film breakup splashed from the blade trailing edge are carried out. Through the investigation on a mechanism for droplet generation on the blade trailing edge, decrease in erosion damage on moving blades in the last stage of steam turbine is aimed.

Material Degradation in High Temperature Water

In order to improve the prediction accuracy of material degradation in power plants, the final goal is set to develop an evaluation method of the degradation on the basis of material surface condition. Oxidation behavior in conjunction with crack embryo formation and reactions at the alloy/oxide film interface is presumed. Process before small crack initiation is investigated under the simulated power plant conditions with special emphasis on surface oxidation and its localization.

Hane/Sasaki Laboratory

Opto-mechanics



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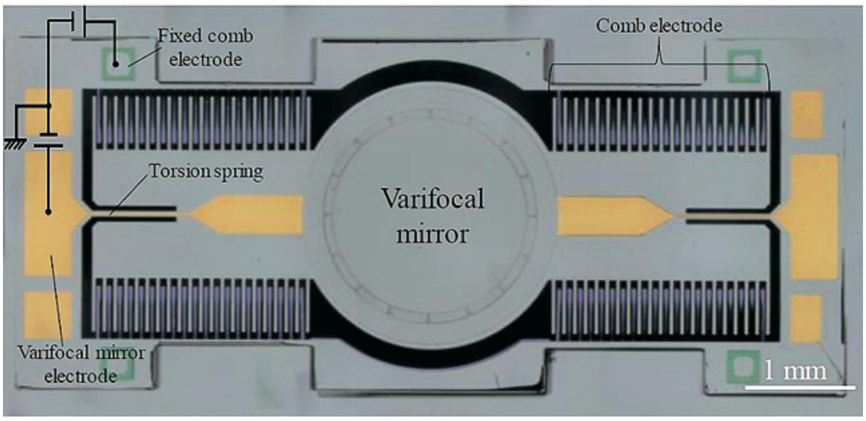
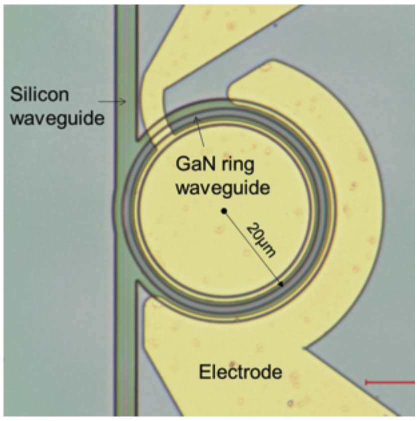


Laser beam scanner with varifocal mirror



GaN micro-ring on silicon submicron-wide waveguide

Micro opto-mechanical devices (sensors and actuators)

Micro opto-mechanical devices are designed and fabricated on the basis of silicon micro machining technology. In laser display, laser beam generates image using a two-axes micro-mirror. Large scan angle and fast scan speed are needed for high resolution. In automotive self-driving, laser range-finder with scanning micro-mirror is useful. Several kinds of scanning micro-mirrors are fabricated for the purposes. Moreover, a number of other opto-mechanical devises are studied. An example is a deformable micro-mirror for wavefront compensation in telescope and microscope. Micro-optics and micro mechanical components are combined to generate new opto-mechanical devices.

Optical switches and filters

Silicon photonics is promising, where optical waveguides and electric circuits are merged on the basis of silicon micro fabrication technology. The waveguides are submicron in width. Introducing ultra-small actuators into waveguide circuits, switches for routing and wavelength selecting can be composed. Several kinds of waveguide coupler switches/filters are studied. Those switches/filters are promising for solving the bottle neck of internet signal traffic in data centers.

Fundus imaging devices

Glaucoma is an important eye-disease due to the increase of aged people. Fundus imaging devices are essential instruments for finding eye-diseases. In order to easily diagnose, smart-glasses-type fundus imaging device is studied. Using scanning micro-mirror with laser light, image is projected onto retina and the reflected light is detected by photodetector in the smart glasses. The optics consists of a confocal system, which has a high efficiency for obtaining reflection image.

Acoustically assisted opto-mechanical devices

Micro acoustic devices are widely used such as microphone and acoustic imager. Small and functional acoustic devices are fabricated by micro machining technology. acoustically resonant mirrors are studied for generating periodic and fast focusing in micro-optical systems such as surface profiler and optical coherent tomography. Micro mirrors with acoustic chambers increase the focal range and scan angle. A high frequency acoustic emitter generates a repulsive force for micro-manipulation.

New materials for opto-mechanics

Although silicon is the main material for micro systems, silicon is not a light source material. GaN is a new light source material and can be combined with silicon devices. Silicon micro optical systems with GaN semiconductor are studied. Examples are an optical encoder with GaN light emitting diode, a scanning micro mirror with GaN light source, and a silicon photonic modulator with GaN micro ring resonator.

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Nanomechanics

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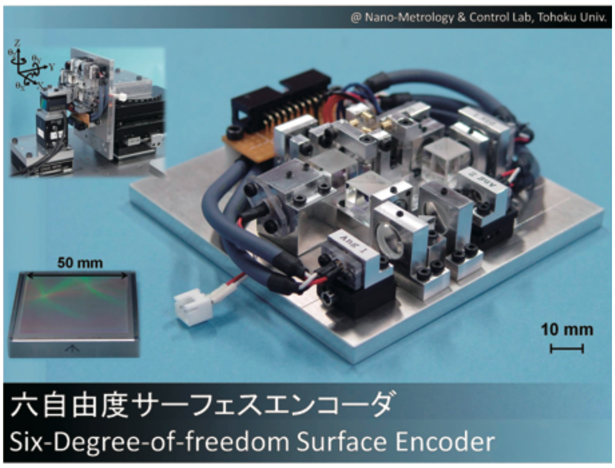

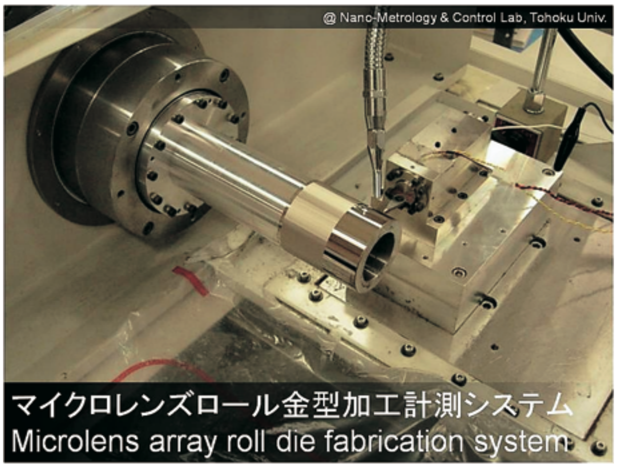

Nanometrology and control of multi-degree of freedom

In our laboratory, we are engaged in research on precision manufacturing measurement that measures the shape of precision processed products and the movement of precision machines with the required accuracy. Based on a unique measurement principle, we have proposed a high precision and compact multi-axis displacement/angle sensor (surface encoder system) which is a basic tool for ultra-precision manufacturing measurement by combining a fine diffraction grating and a wave optical system. This system can detect the position and orientation of six-degree of freedom for high precision positioning systems with a single laser probe.

Scanning probe microscopes for 3D shape measurement

In this study, we have proposed and developed a non-contact electrostatic force microscope for 3D shape measurement. The sample surface is scanned in a non-contact manner while measuring the electrostatic force between the probe bonded to the quartz crystal and the sample surface, where the distance between the probe and the sample is 50 nm or more. The absolute distance between the probe and the sample can be calculated while canceling parameters which affect electrostatic force.

Precision machining and measurement by a fast tool servo

3D fine shapes are used in various fields such as measurement reference planes and microlens arrays. We investigate a 3D fine fabrication method by diamond cutting using a force-sensor-integrated-fast tool servo and an ultra-precision lathe. We have proposed a method which uses the machining tool itself as a measurement probe and uses it for on-machine measurement of the workpiece shape profile.

Stabilized optical angle sensor with a frequency comb

The optical angle sensor based on the laser autocollimation method has a drawback that the sensitivity of the sensor is not stable for a long time measurement because the light spot diameter fluctuates according to the optical frequency fluctuation of the light source. We have been developed an angle sensor that uses a femtosecond laser as a light source and stabilizes the sensitivity of the sensor by utilizing the frequency spectrum of the optical frequency comb.

Study on precision measurement of large roll lathe

The demand for large-area fine shape machining using large roll dies increases. Motion accuracy is highly required for the machine slides of large roll lathes which process dies. In this study, we proposed a system and algorithm to evaluate the straightness error and parallelism error of the driving slide of a large roll lathe separately from the roll mold shape error by using two capacitive displacement sensors.

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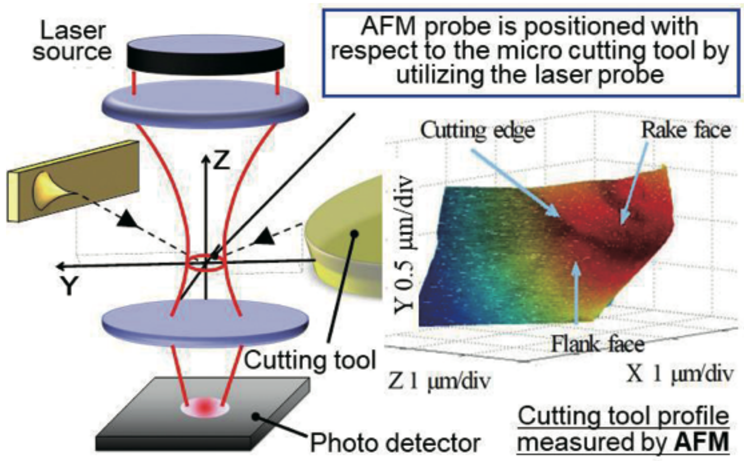
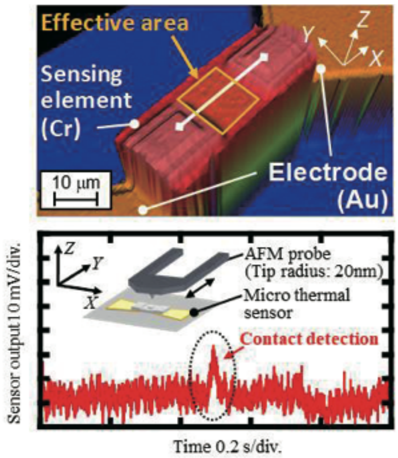


On-machine measurement of a diamond cutting tool



Surface defect inspection by a micro thermal sensor

On-machine measurement of a diamond cutting tool

For the achievement of nanometric ultraprecision cutting, it is necessary to assure the quality of a tool cutting edge. In this research, a compact measurement system based on the atomic force microscopy has been developed. For the fast and precise alignment of the AFM probe tip with respect to a diamond cutting edge under inspection, an optical probe realizing sub-micrometric fine tool positioning has been developed, and quantitative evaluation of the cutting edge profile of a diamond cutting tool has been realized. Furthermore, a method employing the optical probe for evaluation of the tool cutting edge contour has also been developed.

Surface defect inspection by a micro thermal sensor

For next generation LED wafers and magnetic disks, a defect inspection technique capable of detecting small surface defects with a size of tens of nanometer is required. In this study, a new surface defect inspection method, in which a micro thermal sensor capable of detecting the change in heat flow between the sensor and a target surface is employed, has been proposed to carry out surface defect inspection on a flat and smooth surface.

Precision profile measurement of aspheric surfaces

A method for evaluating aspheric surface profiles based on a point scanning method has been developed. In the proposed method, the influence of the motion errors of a linear slide for probe scanning is cancelled by the software-datum method. In addition, a method compensating for the influence of the form error of the probe sphere is also proposed for further accurate evaluation of aspheric surfaces having steep slope surfaces.

A highly sensitive optical angle sensor

The sensitivity of conventional angle sensors based on the autocollimation method is proportional to the focal length of the collimator objective. In this paper, an optical angle sensor based on the laser autocollimation, in which the sensor sensitivity becomes independent from the focal length of the collimator objective, has been developed. The compact angle sensor designed in a size of 26×22×12 mm has achieved a measurement range of ±30 arcsecond and a resolution of 0.05 arcsecond.

Development of a micro-XY stage

For the precision positioning of small components, a micro-XY stage having a long stroke along the in-plane directions has been developed. The stage system has achieved smooth motion by the employments of SIDM method that can be realized by a permanent magnet and a PZT actuator. A Cr-N displacement sensors, which are fabricated by directly patterning strain gauge elements on the leaf springs of the stage system, have also been employed to achieve further higher precision positioning.

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Nanomechanics, Mechanics of Materials System

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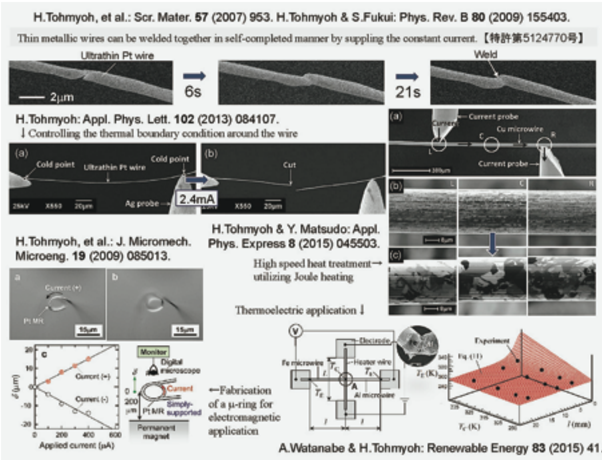
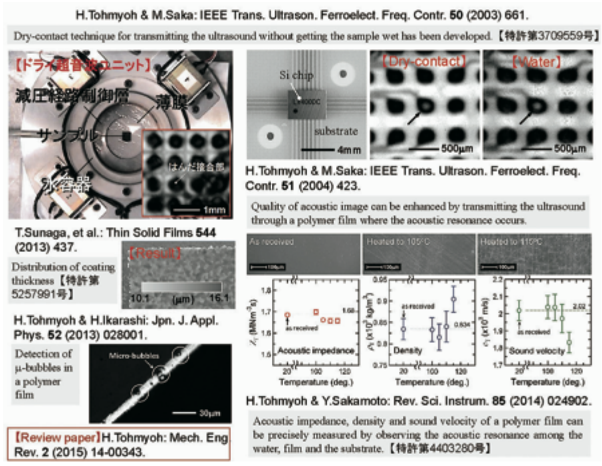


Joining and structual modification of metallic thin wire by Joule heating



Advanced ultrasonic materials evaluation utilizing acoustic resonance

Joining and modification of fine-scale materials by Joule heating

We aim to create an advanced materials system with interdisciplinary approach (Fig.1). To freely use micro/nano materials, which have excellent physical properties and unique geometrical features, techniques for joining and structural modification of such fine-scale materials have been developed. When the constant current is supplied to the contacting portion of metallic wires, the portion is melted by Joule heating and then solidified. By discovering the governing parameter for this phenomenon, two wires were welded together with higher probability. Crystalline structure of thin wire is modified by Joule heating to recover its formability.

Thermoelectric power generation from a thin plate

Thermoelectric function has been created from thin plate or wire. A plate-type thermoelectric power generator has been developed for power generation from a small temperature difference, and the bi-metal interface was realized by depositing Al layer on the surface of the Fe plate. It has been clarified that oxidizing the bi-metal interface is effective to enhance its performance. Moreover, thermoelectric microwire was fabricated for temperature sensing at a local region.

Advanced ultrasonic materials evaluation

A dry-contact ultrasonic technique has been developed for realizing the ultrasonic imaging of an electronic device without getting the device wet (Fig.2). Here the high frequency ultrasound is transmitted into a sample via a thin film inserted between the water and the sample. Moreover, layered media, such as polymer film and coating, were successfully characterized utilizing the acoustic resonant phenomenon, which occurs when ultrasound passes through a thin layer.

Mechanical testing of micro/nano materials

For creating an advanced materials system from fine-scale materials, understanding the various physical properties of such materials is vital. For evaluating the mechanical properties of micro/nano materials, a force sensor for measuring the micro-Newton force has been developed, and the mechanical testing of micro/nano materials is performed. Moreover, electrical properties of micro/nano materials are evaluated by eddy current microscopy or small-scale potential drop technique.

Characterization of human hair and nail

Human hair and nail have been found to hold various information on our disease and aging, and therefore it is expected to be used as a specimen for medical diagnostics like blood or urine in the future. For this purpose, the deformability of such biomaterials was examined by bending and tensile tests, and the effects of water absorption and inclusion of a metal ion on their deformability were investigated. Moreover, we are investigating the factor deciding the shape of a human hair.

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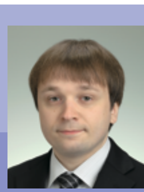

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Molecular Heat Transfer Laboratory

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Specially Appointed Assist.Prof.
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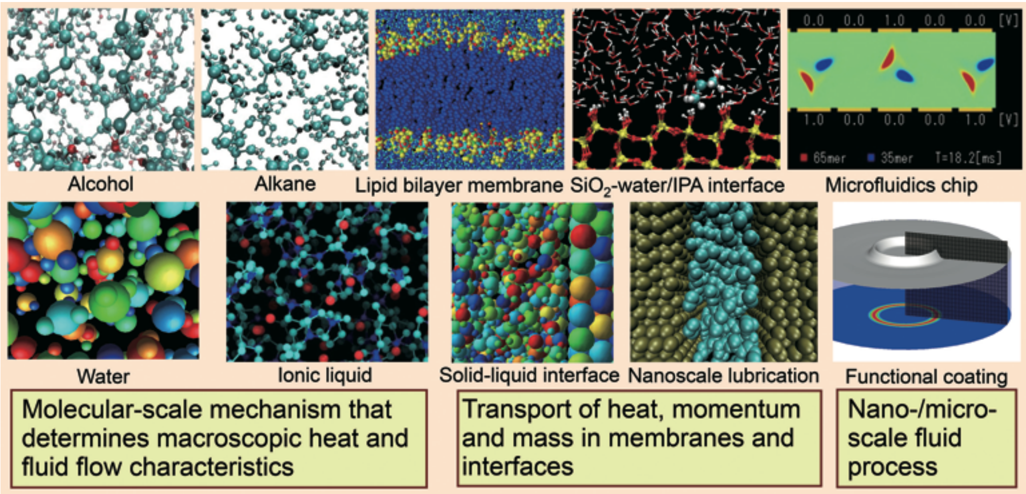

Molecular Thermal and Fluids Engineering

Analysis of thermal and fluid phenomena based on the molecular dynamics theory leads to understanding of fundamental mechanism of the phenomena, and ultimately, to the design of thermal and fluid phenomena that are needed in the cutting-edge area in modern technologies. Also the molecular-scale analysis is effective for thermofluid phenomena in extreme conditions in which macroscopic models such as thermophysical properties and the concept of interface are no longer valid. The molecular heat transfer laboratory is engaged in the research to analyze nanoscale thermal and fluid phenomena, from the molecular scale to the MEMS/NEMS scale, and the applications.

Fluid Structure and Transport of Energy and Momentum

Liquids contain various structures which govern transport phenomena of mass, momentum and thermal energy. Analysis of liquid structures and their transport characteristics gives a thorough answers for some questions such as why the liquid have its specific value of thermophysical properties and how the molecular structure should be to realize a liquid having desired thermophysical properties. Anisotropic transport in heterogeneous soft matters are also analyzed to seek novel materials.

Heat and Mass Transfer at Solid-Liquid Interfaces

Heat and mass transfer at solid-liquid interfaces governs overall characteristics of nano-structured systems such as NEMS, semiconductor devices and porous materials. Molecular dynamics simulation analyzes mechanisms of thermal energy transfer over the interface and mass transfer in the anomalous structures in liquids in the vicinity of solid surfaces Basic studies to seek molecules and nanostructures which exhibit required interface characteristics are also performed.

Design of Novel Thermal Fluids Based on Molecular Data

Thermal fluids plays a major role for highly efficient usage of thermal energy in sophisticated thermal devices. The aim of this study is to know the structure of molecules for thermal fluids which are optimized for specific conditions and give the best performance. This is accomplished based on the data concerning thermal energy transport in fluids, which are obtained by analyses of mechanical energy transfer due to dynamic motions of molecules and functional groups in molecules.

High-Functionality Coating

Coating is a complex application technology where liquid-gas/solid-liquid interfacial phenomena and micro/nanoscale fluid flow are coupled. Requirement for coating of molecular-scale film thickness is getting severe in these days; Alignment control of coating film molecules and dynamic coating based on adsorption and disorption of surface-covering molecules are the examples. Molecular thermofluid analysis is applied to solve the problems to achieve fine and highly functional coatings.

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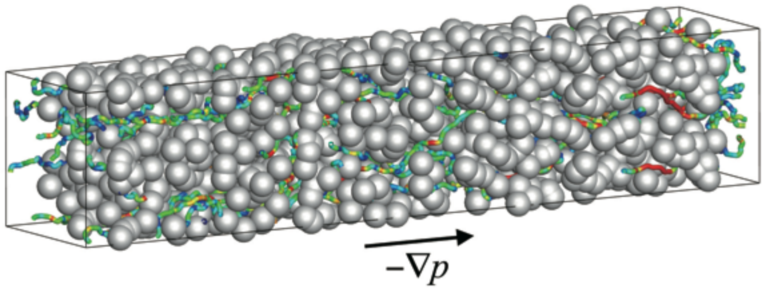
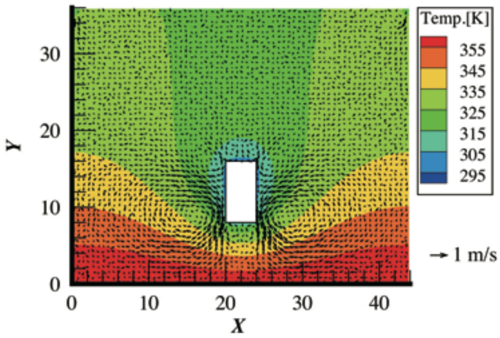


Streamlines of micro/nanoscale gas flow through a porous medium induced by applied pressure gradient



Gas flow induced around a microscale object immersed in a gas with non-uniform temperature

Study on Molecular Gas Flow

In rarefied gas flows, cold plasmas, and micro/nano gas flows, mean free path of molecules is comparable with characteristic lengths of gas flows. Such flows are in strong nonequilibrium due to lack of intermolecular collisions and cannot be considered as a continuum. Therefore, they have to be treated in view of atoms, molecules, ions and electrons, and hence, are termed molecular gas flows. In such flows, the effect of gas-surface interaction becomes large, and hence, phenomena such as thermal creep and Knudsen force can occur, which are not shown in usual continuum flow. We study the phenomena of such flows and use the knowledge obtained here in industry.

Molecular Gas Dynamics Study on Nano Gas Lubrication

The friction coefficient of a partially polished diamond coating drastically decreases as sliding speed increases. Using theoretical analysis, we clarified its mechanism as follows: High gas pressure is induced by the presence of dimples. Then, it separates two sliding surfaces, and leads to the situation where both surfaces are non-contact. This is the reason of low friction. This lubrication system can be applied to any mechanical devices with sliding parts such as bearing system.

Study on Micro/Nanoscale Gas Flow in Porous Media

In porous media with nanoscale pore used in fuel cell, peculiar phenomena such as velocity slip and Knudsen diffusion appear. Due to those, it is difficult for us to evaluate gas flux because its permeability is affected by them. The objective of the present study is to clarify transport phenomena in such porous media from the viewpoint of molecules. So far, we proposed and verified a theoretical expression, which gives gas flux and permeability in the whole range of Knudsen number.

Study on Non-Coalescence of a Droplet and a Liquid Pool

It is considered that if a liquid droplet is dripped onto a pool of the same liquid, they will immediately coalesce. But, in reality, it is often seen that a dripped droplet floats on a liquid pool for a while without coalescing. In the present study, we clarify the mechanism of this noncoalescence by focusing on the role of micro/nanoscale gas flow between two facing liquid surfaces.

Study on Knudsen Force Due to Non-Uniform Temperature

When the gas temperature changes within a length scale as small as the mean free path of gas molecules, an object immersed in such a gas is subjected to a force from the gas. On the other hand, the gas is also subjected to its reaction force and starts to flow. This force is called Knudsen force and cannot be seen in usual length scale. The objective of the present research is to clarify and understand the Knudsen force, and then to apply it to transportation of microscale object.

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Molecular Composite Flow Laboratory

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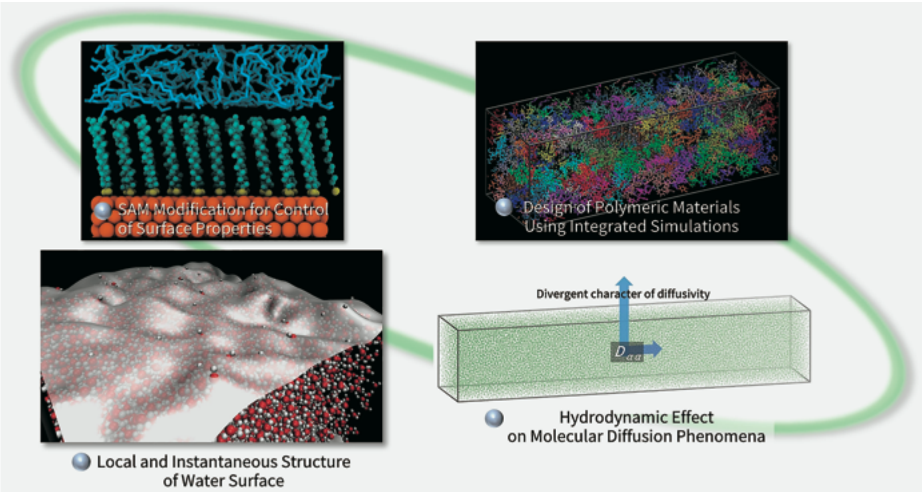

Molecular Composite Flow Systems Studied by Molecular Simulations

Molecular Composite Thermal and Fluid Phenomena

From nanoscale to macroscale, various thermal and fluid phenomena, to which composite molecular-scale physics gets engaged, are of critical importance in the wide range of engineering and industrial processes. By using large-scale numerical simulations such as the molecular dynamics method, we investigate heat and mass transport phenomena emerged in the thermal and fluid engineering from the microscopic viewpoint. Integrating numerical analysis methods which can cover multiscale physics and data analysis based on machine learning, we aim to investigate thermal and fluid phenomena having multiscale aspects.

Surface Modification Using Organic Molecular Films

Novel surface modification techniques at the molecular level such as the self-assembled monolayer (SAM) have drawn attention as techniques to control the physical and chemical properties on solid surfaces. Structure formation, interface affinity, and heat and mass transport characteristics of organic molecular films have a critical importance in the engineering and industry. We investigate the underlying microscopic mechanisms of these significant characteristics.

Thermal and Fluid Properties of Polymeric Materials

As for development of polymeric materials which have extensively been utilized in industry, designing thermofluid properties as well as mechanical and chemical properties by controlling the molecular-scale structure and phase separation structure inside the material is being required. Using integrated numerical analyses covering molecular-scale to macroscale phenomena and data-driven informatics techniques, we aim to explore and design novel polymeric materials.

Transport Phenomena in Confined Liquids

At the fluid and soft matter interfaces or inside the confined liquid in nanoscale structures, peculiar heat and mass transfer characteristics emerges as a consequence of heterogeneous structure formation inside a liquid in the vicinity of the interfaces. Our goal is an essential understanding of heterogeneous structure and corresponding transport phenomena at the molecular level, which is significantly different from that in homogeneous bulk media.

Hydrodynamic Effect on Molecular Diffusion Phenomena

Molecular diffusion phenomena are directly relevant to the wide field of nano- and bioengineering, e.g., molecular transport through mesoporous materials and biomolecules. It is well known that the molecular diffusion is highly affected by the hydrodynamic effect induced by the molecule itself. We lead the fundamental study on the mass transport phenomena bridging between macroscopic fluid dynamics and molecular dynamics.

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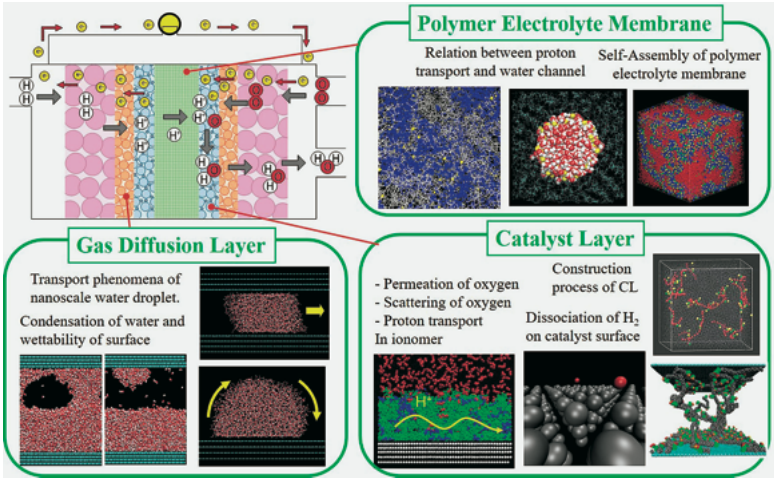
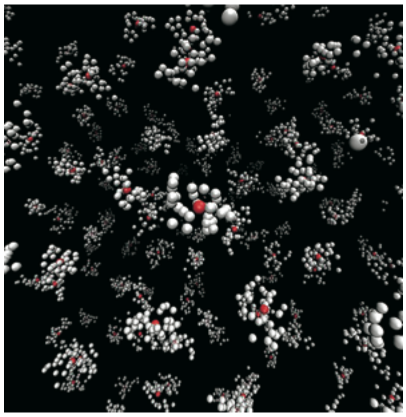


Molecular dynamics simulations of mass transport phenomena inside a polymer electrolyte fuel cell



Schematic diagram of hydrogen molecules considering quantum effects by path integral method

Analysis of nanoscale flow phenomena including quantum effect

There are many flow fields, in which quantum effects of atoms affect the flow properties. For instance, because hydrogen has large uncertainties of position and velocity due to its light molecular mass, the conventional molecular models cannot be applied. Moreover, protons diffuse in liquid or solid much faster than water molecules because of the additional transfer mechanism involving a chemical reaction, which is the formation and concomitant cleavage of covalent bonds. In our laboratory, we treat the systems including the quantum effects of molecular fluid by various methods, and find out its physical mechanisms to apply the results to engineering aspects.

Transport phenomena in polymer electrolyte fuel cells

Polymer electrolyte fuel cell (PEFC) is a promising next-generation power supply system that generates electricity by reacting hydrogen with oxygen. To improve its efficiency, it is important to transfer efficiently reactants and products. However, the flow filed is constructed by very fine structures in micrometer or nanometer. In our laboratory we investigate the transport phenomena of small molecules in the materials in PEFC by large-scale molecular dynamics simulations.

Analysis of transport properties of hydrogen in solids

In the flow phenomena of hydrogens, hydrogen molecules have quantum effects unlike other atoms due to its light molecular mass. Thus, it is difficult to describe the hydrogen flow phenomena by using conventional classical molecular dynamics methods. In this study, we explore how the quantum effects of hydrogen affect its thermal flow characteristics using a special technique to take into account the quantum effect in the framework of molecular dynamics, and apply these techniques to numerical prediction of transport phenomena of hydrogen in solids.

Analysis of oxygen ion transport in ceramics

In solid oxide fuel cells, oxygen ions move inside the ceramic electrolyte from cathode to anode to proceed the reaction. If this oxygen ion transport property is improved, efficiency and operating temperatures can be improved. In this study, we analyze the transport properties of oxygen ions inside the ceramic electrolyte using molecular dynamics method, aiming at the theoretical design of electrolyte ceramics which has advanced transport efficiency of oxygen ions.

Reactive molecular dynamics study on film formation

In semiconductor manufacturing, the film formation process requires atomic layer level control with film thickness error less than ± 0.5 mm. Chemical vapor deposition and atomic layer deposition methods are widely used as film deposition techniques that can meet such cutting-edge demand. In this study, we aim at a universal understanding of the deposition mechanisms using the reactive force field (ReaxFF) molecular dynamics simulations that merge the diffusion and reaction phenomena.

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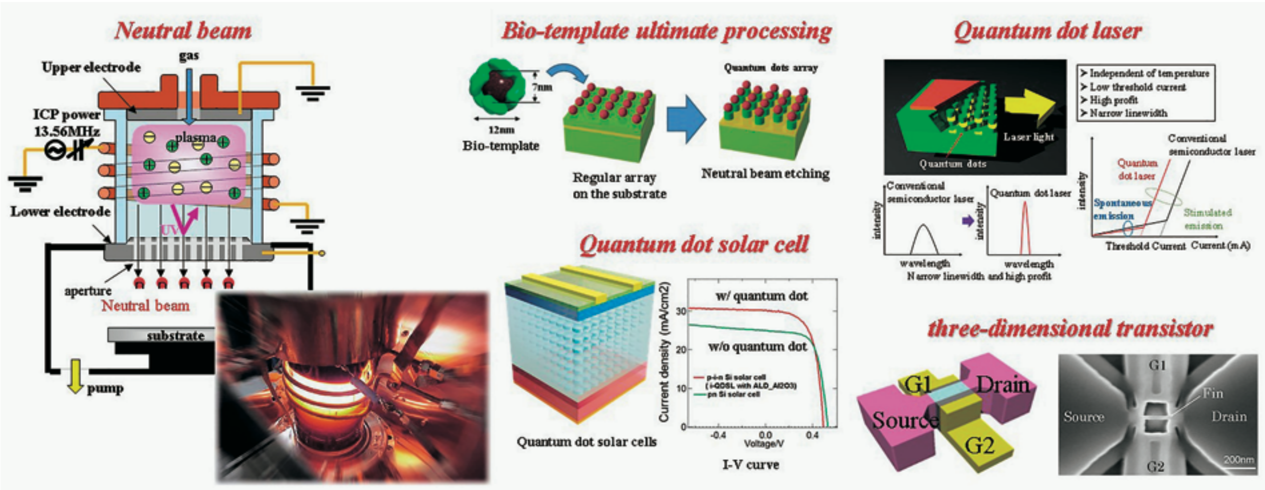

Innovative green nanodevice development by ultra-low damage process

Semiconductor device technologies such as VLSI and quantum dot solar cells will need support devices and connected home appliances being developed in the IOT revolution. These devices need to be fabricated by thin film material deposition and damage prone processing technologies using high energy ions, electrons and photons. A key technology in our laboratory is a defect-free neutral beam process. By combining this with our research on a completely new, innovative green (ultra-low power) bio-template processing technology, a highly precise, uniform, defect-free, and well-aligned quantum dots structure can be fabricated with customizable size and density.

Solar cells/thermoelectric elements

Our unique bio-template processing in conjunction with neutral beam technology is able to produce the world's first well-aligned, high-density quantum dot structure arranged over a large area. Thanks to this, the devise bandgap can be tuned leading to the design of ultra-high efficiency solar cells. In addition, quantum nanostructures can control phonon scattering characteristics. This property can help design ultra-high efficiency thermoelectric conversion elements.

Quantum dot laser/light emitting device

III-V compound semiconductor quantum dot lasers are the expected light source for next generation that are temperature-independent, ultra-high speed, low power optical communications. This is the reason why the technology to control the size of quantum dots without any defects is indispensable. In our laboratory, we have developed an ideal quantum nanodisk structure by bio-template extremely precise processing and are currently developing a compound semiconductor laser using it.

Advanced high-speed MOS transistors

In the latest electronic circuits, three-dimensional transistors have been introduced to further improve performance. However, conventional manufacturing methods cannot provide sufficient performance due to process-induced defects. We have succeeded in greatly improving transistor performance by using processing and surface modification with a damage-free neutral beam source. In addition, we are developing transistors with new materials such as Ge.

Applications of surface treatment process

Neutral beams are extremely effective for nanoscale surface treatment processes. High-quality gate oxide and metal oxide films necessary for next-generation germanium transistors in resistance-change memory, one of the latest random-access memory types, are achievable using an oxygen neutral beam. Moreover, low damage etching and selective synthesis is possible by irradiating graphene with the neutral beam of oxygen and nitrogen.

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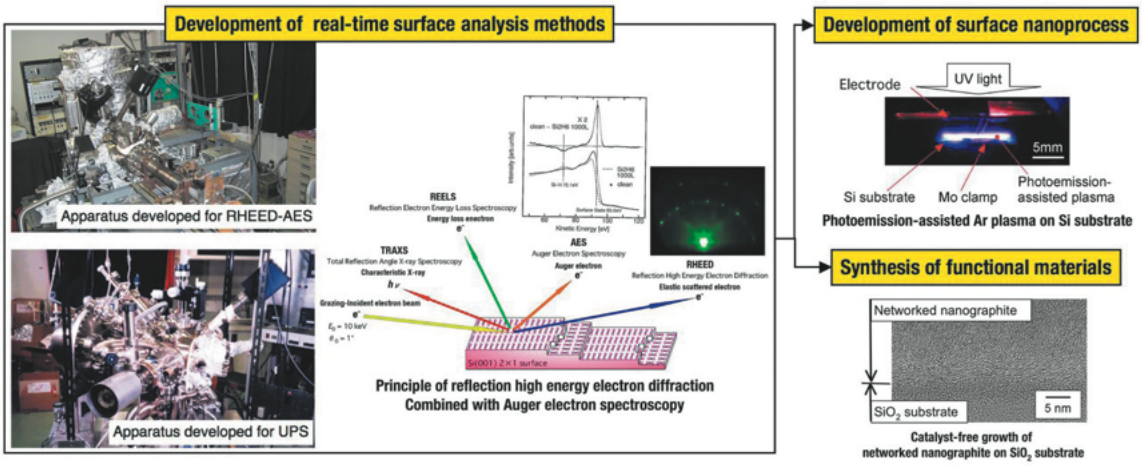

Functional thin film synthesis and surface nanoprocess development based on understanding of solid surface reaction mechanisms

Development of real-time material surface measurements

Our laboratory is developing functional materials and developing surface nanoprocesses based on the understanding of surface/interface reaction mechanism, with the basic policy of developing and applying new surface physics measurement methods. In addition to research to connect the seeds obtained by elucidating the surface reaction mechanism to the needs of industrial applications, we will discover the problems required of surface science from the needs of industrial applications. In order to achieve this, a boundary area between basic and applied or a research subject of science and engineering is set.

Vapor phase synthesis process of nanocarbon materials

In order to efficiently deposit nanocarbon thin film materials only on the substrate surface, we are developing a "photoemission-assisted plasma CVD process" that controls direct current discharge using photoelectrons emitted from the substrate surface irradiated with ultraviolet rays. Currently, this process is being used to develop diamonds for low friction coefficient diamond-like carbon, low resistance carbon materials for wiring, and heat spreaders for IC chip cooling.

Study of CMOS gate insulating film formation mechanism

We are researching the mechanism and reliability of insulating film SiO_2 formation for next-generation CMOS gate stacks, focusing on the oxidation-induced strain generated during the Si oxidation reaction. We are proposing an "Unified Si oxidation reaction model" that can complementarily explain the growth, decomposition, and reliability of SiO_2 films by using point defect generation, and are conducting model verification experiments.

Development of nano-level surface planarization process

Photoemission-assisted plasma can also be used as an efficient low energy ion source. Taking advantage of this feature, we aim to develop an inch-size metal surface flattening process. At present, the surface roughness of a copper substrate having an initial roughness Ra = 1 nm has been successfully reduced by about 20%. In the future, we plan to develop a planarization process aiming at 0.1 nm equivalent to one atom, and to planarize non-metallic surfaces such as diamond.

Study of molecular adsorption on catalytic surface

The our unique real-time photoelectron spectroscopy can simultaneously measure the amount of molecular adsorption on the metal surface and the work function. Since the orientation of adsorbed molecules can be examined from the work function, the reaction path of the adsorbed molecules can be examined. Utilizing this technique, we are promoting the development of catalysts that render toxic gases harmless and research to produce hydrogen from hydrocarbon gases.