Program

International Symposium & School on Crystal Growth Fundamentals

"New Insights into Crystal Growth Fundamentals:

A tribute to Profs. Ichiro Sunagawa and Pieter Bennema”

November 3-7, 2018

Convention Hall of Hotel Sakan, Akiu, Sendai, Japan

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Taketoshi Hibiya

Keio University

Memory of Piet Bennema for the discussion of garnet morphology on a boat

I met Prof. Bennema in Stuttgart, Germany, where the ICCG-7 was held. I presented a paper on morphology control for liquid phase epitaxial growth of magneto-optic iron garnets. During the conference a boat excursion was held along the Marbach am Neckar. On boat Prof. Bennema and I talked lots about morphology of garnets; at that time he was engaged in calculation for periodic-bond-chain of crystals in particular for the garnet system and I was faced to difficulty in morphology control of garnets. I learned from him not only the latest scientific research result but also his experience in Indonesia during the Second World War.

Jim De Yoreo

Pacific Northwest Laboratory

Classical vs non-classical pathways of crystal nucleation and growth

Recent observations have shown that crystallization occurs along a rich set of hierarchical pathways involving species of higher order than simple monomers, ranging from multi-ion clusters to dense liquid droplets to transient amorphous or crystalline particles. The extent to which these pathways can be understood using well-known concepts of classical nucleation theory or require alternative “non-classical” models is a matter of current debate. Here I use a number of examples from in situ AFM and TEM studies of nucleation and growth to illustrate the diversity of pathways seen during crystallization and provide a holistic picture of that relates non-classical dynamics to classical concepts.

Geun Woo Lee

Korea Research Institute of Standards and Science

Crystal nucleation and growth in a deep metastable liquids using electrostatic levitation and dynamic diamond anvil cell

We develop a novel device, a combination of electrostatic levitation, and x-ray and Raman scattering, so that we can achieve extremely high supersaturated solutions, and its atomic and molecular structure and thermodynamics. Using this new device, here, we will demonstrate that a levitated KH_2PO_4 (KDP) aqueous solution shows two different nucleation paths with the degree of supersaturation, while $(NH_4)H_2PO_4$ (ADP) solution (a family materials with KDP) does not. Moreover, by measuring molecular structure and its evolution in the highly supersaturated solution prior to nucleation, we find a solution-solution transition in short range order which underlies the different nucleation path.

4(Sun.)8:00

Juan Manuel García-Ruiz

CSIC-University of Granada

Patterns on the rocks: An overview of mineral growth patterns

Understanding howcrystals, their morphology and their texture are related to growth conditions is the gate to revealingbygone geochemical environments when no other proxies are available. In this lecture I invite you to join me on a personal journey through rock patterns, from those controlled by the mineral crystal structure, as those currently forming giant crystals of gypsum, to patterns with non-crystallographic symmetry, as those controlled by interaction of transport and chemical precipitation leading to mineral self-organization.

4(Sun.)8:40

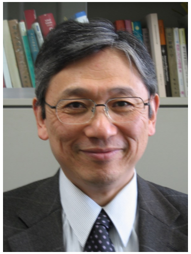
Teruki Sugiyama

National Chiao Tung University

Crystallization controlled by optical trapping

Optical trapping in solution increases solution concentration locally at laser focus, triggering spatiotemporally-controlled crystallization. Ever since we firstly succeeded in demonstrating optical trapping-induced crystallization of an amino acid in 2007, we have explored novel optical trapping-controlled phenomena such as crystal growth and polymorphism for amino acids and proteins. In this presentation, we will first make a brief introduction of the principle of optical trapping and then present these research results. In addition, recent results about chirality control in chiral crystallization utilizing plasmonic optical trapping will be also presented.

4(Sun.)9:40



Koichi Kakimoto

Kyushu University

Numerical investigation and experimental validation of crystal growth of semiconductors

This paper reports the synergy effect of both experimental results and numerical validation on crystal growth of semiconductor crystals. The paper contains quantitative comparison between experimentally obtained defect density and numerically calculated data in semiconductor crystals. The paper also contains the results on interface shape and stress distribution in a growing bulk crystal. The quantitative discussion will be discussed based on the experimental and numerical results.

Elias Vlieg

Radboud University

Structures of interfaces

The growth of crystals takes place at the interface with its growth medium and (nearly) always atom by atom (or molecule by molecule). A complete understanding of crystal growth therefore requires an atomic-scale knowledge of the processes and structure at the interface. At the growth interface, both the crystal and the growth medium will typically have a structure that is different from the bulk. Assessing such interfaces, in particular when growing from a solution or melt, is quite difficult, but a combination of techniques like AFM, computer simulations and X-ray diffraction, has yielded significant insights.

4(Sun.)11:20

Takeshi Fukuma

Kanazawa University

Visualizing atomic-scale structures and dynamics at solid-liquid interfaces by high-speed frequency modulation AFM

Atomic force microscopy (AFM) has been widely used for imaging nanoscale step flows during crystal growth and dissolution. However, it has been difficult to visualize atomistic events at the step edges. To overcome this limitation, we recently developed high-speed frequency modulation atomic force microscopy (FM-AFM) and imaged atomistic events at the step edges during the calcite dissolution. These images revealed the formation of $Ca(OH)_2$ monolayer along the step edges as an intermediate state of the dissolution. In this lecture, I will overview the recent progress in the development of in-liquid FM-AFM and its applications to crystal growth studies.

4(Sun.)14:00

Teruyasu Mizoguchi

University of Tokyo

Machine learning for atomic-resolution analysis of interface

Interface plays important roles for materials properties, such as mechanical strength, electric conductivity, and crystal growth. Thus, the modeling of the interface structure is one of the most important subjects for the materials research. On the other hand, the modeling the interface is usually difficult due to its geometrical freedoms. Here, we have applied machine learning techniques to accelerate the interface structure determination. I will talk on our method, virtual screening, kriging and transfer learning, for the interface structure searching, in my presentation.

4(Sun.)14:40

Qiu-Sheng Liu

Chinese Academy of Sciences

Solutal convection of liquid in alloy directional solidification with porous dendrite mush

Alloy solidification commonly takes place with a cellular or dendritic microstructure, i.e., with a region of intimately co-existing liquid and solid phase named as "the mushy layer". During alloy solidification, there always exists a mushy layer sandwiched between pure liquid and solid phases. In this lecture, theoretical study of the onset of solutal convection during the directional solidification of Bridgman type on liquid Al-3.5wt%Li is presented. In the double-layered system where the liquid layer on the top of mush is considered, the depth ratio and the porosity at the liquid-porous interface are both relevant with the pulling rate. A mode transition between the two modes of instability convection is also predicted to occur under the increase of pulling rate, which varies the depth ratio together with the permeability of the porous layer.

4(Sun.)15:40

Toru Ujihara

Nagoya University

Machine learning for SiC crystal growth (modeling, optimization and visualization)

In this study, we constructed prediction model of CFD result by using machine learning technique as follows: (1) we prepare 300 results of CFD simulations as training data for machine learning and (2) we produce the prediction model on neural network. Figure 1 shows the simulation result of supersaturation distribution and fluid velocity distribution and the predicted result based on the prediction model. Surprisingly, both results are very similar to each other. Moreover, the average calculation time of the simulation and that of the prediction model are about 3000 s and 0.003 s, respectively. Using this prediction model, it is also possible to decide an optimized condition

4(Sun.)16:20

Noriko Akutsu

Osaka Electro-Communication University

Introduction to deep learning with a software Keras: A guide for end-to-end users

Deep learning has led to remarkable achievements in recent years. It offered better performance on many problems. Deep learning also makes problem-solving much easier, because it automates feature engineering. By this automation, machine-learning workflows are simplified from the multistage pipelines to a single end-to-end deep-learning model. In addition, the rise of user-friendly libraries such as Keras is driven by TensorFlow which is a tensor-manipulation framework for Python. In order to apply this new method to our own problems, a guide of the software Python with Keras for end-to-end users is shown.

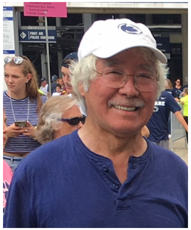
4(Sun.)17:20

Hiroaki Imai

Keio University

Formation of mesocrystal: classical and non-classical crystal growth

Sophisticated architectures consisting of oriented small crystalline blocks are observed in biological and biomimetic minerals. Recently, these hierarchical structures are categorized into mesocrystal as intermediate between single crystals and polycrystals that are random arrangements of small grains. Here, artificial formation processes of mesocrystals are discussed on the basis of the growth mechanism. Various hierarchical crystalline architectures are constructed through classical routes including nucleation and growth that are controlled by organic agents. Several mesocrystals are also produced through nonclassical routes including oriented attachment of specific nanoscale blocks.



Hiroshi Ohmoto

Pen State University

New model for the condensation of minerals in the Solar Nebula and the origin of Earth based on the meteorites discovered in 3.46 Ga-old submarine basalts

Geochemists have estimated the bulk compositions of the early Solar System and of the Earth from the compositions of: (1) meteorites (e.g., CI chondrites) that have fallen on Earth during the past ~300,000 yrs, and (2) the present-day Solar Winds. Yet, the possibility that the early Solar System had significantly different composition than these materials has not been questioned. Based on the results of mineralogical, geochemical and geological investigations of the recently discovered 3.46 Ga-old meteorite fragments in Australia, I will discuss a new model for the Earth formation.

5(Mon.)8:40

Noriaki Ozaki

Akita Prefectural University

Silica biomineralization in rice plants

Biogenic amorphous silica (biosilica) is widely found in diatoms, marine sponges, some higher plants and bacteria. Biosilicas in diatom and sponge, are formed under mild condition and neutral pH using organic matrices (unique proteins and long-chain polyamines). Although rice plants produce large quantity of biosilica in their leaves and rice hulls, the molecular mechanisms of silica biomineralization is still unclear. Here we report some preliminary results on the characterization of several proteins, extracted from the biosilica of the rice plants (Oryza sativa). As far as we know, this is the first report of protein identification existed within biosilica of the rice plants.

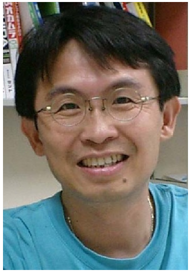
Chaorong Li

Zhejiang Sci-tech University

Morphology control and applications of Cu_2O nano-particles

Cu_2O has many applications in photo-electronic areas. The morphology of Cu_2O nanoparticles plays important role in their property performance. For instance, different crystalline surface shows different catalysis behavior, due to their different surface energy. In this talk, we will shall how to obtain cubic, octahedral, truncated cubic and truncated octahedral morphologies by some simple controlling ways during fabrication, and then investigated their properties and introduce several applications of the fabricated Cu_2O nanocrystals.

5(Mon.)10:20

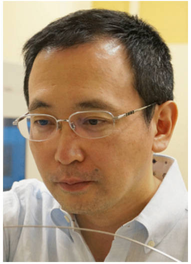


An-Pang Tsai

Tohoku University

Growth of quasicrystals

Quasicrystals display diffraction patterns with symmetries forbidden in crystallography, and quasi-periodicity, have been found to be stable phases in several alloy systems. Thanks to their stability, one can grow single grained quasicrystals with large scale. In this talk, we will first make a brief introduction to quasicrystals and describe the state of the art of structure for icosahedral quasicrystal. The morphologies of icosahedral quasicrystals are discussed in terms of atomic structures, surface structures and crystal growth mechanism.



Michihiko Nakamura
Tohoku University

Magma crystallization and volcanic eruptions

In volcanic eruptions, crystallization of magmas is driven by decompression-induced degassing rather than by cooling. Groundmass microlites record magma ascent rate from the magma reservoir to the shallow conduit, which is a fundamental factor controlling eruption explosivity. However, microlites do not record the explosive-effusive transitions in some eruptions, when such transitions are governed by the decrease of exsolved volatile pressure in the shallow conduit. Instead, the difference in the slope of crystal size distributions (CSDs) down to 1 nm among the eruption styles may be interpreted by considering the difference in magma residence time and fragmentation pressure.

Etsuro Yokoyama

Gakushuin University

Morphology, roughening and instability

This talk is focused on the stability of a growing interface and the relation between the stability and interface structures, such as kinetic roughening and smooth interface. For example, a growing ice disk in supercooled water has two distinguish instabilities, in which growth of the radius is controlled by transport of latent heat, on the other hand, disk thickening is governed by the generation and lateral motion of steps on the basal faces. The morphological instability occurs at the edge of the basal face, while the instability of facet occurs on the basal face. We discuss the difference between morphological instability and facet instability.

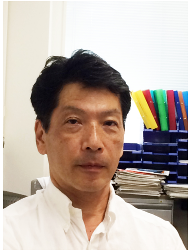
Yuki Kimura

Hokkaido University

Application of liquid TEM to various crystallization

Transmission electron microscope (TEM) is a powerful tool to observe a material in nanoscale. Unfortunately, however, there is some limitations on a sample. Particularly, samples must be dry, because it is exposed to a vacuum environment in TEM. Therefore liquid samples are not able to observe as is. Recent years, several techniques using MEMS liquid cell, graphene cell and ionic liquid have been developed to observe liquid samples. Here, I will introduce several techniques and example results, such as nucleation and growth of several nanoparticles including behaviors of defects, a concretion process and dissolution processes.

5(Mon.)17:20



Junpei Yamanaka

Nagoya City University

Self assembly of colloidal particles

Uniformly shaped colloidal particles dispersed in liquid media self assmble into ordered crystal structures. We introduce crystallization in various colloidal systems, including hard sphere systems, charged colloid, and depletion attraction systems (colloid + polymer). In the hard sphere colloids the crystallization is purely entropic. The charged colloids crystallize due to electrostatic repulsion between the particles, while the driving force of the depletion system is an attraction due to difference in osmotic pressures between those in bulk and in a gap of two particles. We also report clustering of small number of colloidal particles, and further clustering of the clusters.

6(Tue.)8:00

Mu Wang

Nanjing University

The mechanism leading to the long range ordering in the interfacial aggregation

Nucleation is an important step in crystallization, and many self-organized patterns are mediated by the very unique spatial environment for nucleation process. Here we take some examples to show the significance of concave-corner-mediated nucleation in both self-organized formation of long-range-ordering crystalline structures and in self-assembly of metallic nano wire arrays.

Xiang-Yang Liu

National University of Singapore

Kinetic and control of spider silk crystallization

To re-engineer the hierarchical structure of soft materials， ie. silk fibroin, and to functionalize the materials can be achieved by controlling nucleation at the mesoscale. In this talk, I will cover the principles and strategies of mesoscopic structural re-engineering and functionalization of silk fibroin materials based on Intra/inter molecular nucleation. This allows in the design and integration of high-performance bio-integrated devices for future applications in consumer, biomedical diagnosis, and human–machine interfaces.

6(Tue.)9:40

Tetsuo Okutsu

Gunma University

Light induced crystallization of proteins and organic molecules

We discovered a phenomenon in which protein crystallization is induced by surface plasmon resonance, and elucidated its mechanism. Protein molecules adsorb onto the surface of gold nanoparticles with high density. Molecules present in gaps between gold nanoparticles are trapped by the electric field of light and stay for a certain time. There another protein molecule is carried in by diffusion and forms a cluster. In this state, when a covalent bond is formed by photochemical reaction using quinone, a tetramer of protein is observed. Nucleation requires time to gather certain molecules, and plotting nuclear appearance against light irradiation time gave a relation indicating induction time.

6(Tue.)10:40

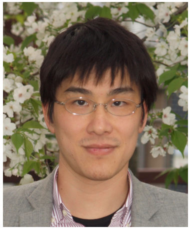
Satoshi Uda

Tohoku University

Growth of new congruent oxide crystals with extended stoichiometric compositions

The new concept of stoichiometry is discussed. The unity of activity for all constituent elements is essential to a material being stoichiometric since the unity of activity leads to zero mixing term in chemical potentials. The activity of an element to be unity needs the standard-state chemical potential equal to the chemical potential itself and one degree of freedom is basically required for each of constituent elements. The degree of freedom is examined for each crystal site by the subtraction of number of constraints from that of constituent elements. Based on the new stoichiometry, we have developed MgO-doped $LiNbO_3$ and $LiTaO_3$ that is simultaneously congruent and stoichiometric.

6(Tue.)11:20



Hitoshi Miura

Nagoya City University

Fundamentals of step dynamics

Surfaces of polyhedral crystals may seem flat by naked eye, but they are not perfectly flat and take some structures in atomistic scale. When the crystal grows, the growth units such as atoms or molecules are incorporated into the surface structure. The incorporation kinetics determines the rate of crystal growth. Therefore, you should learn the incorporation mechanism in order to understand crystal growth. In my lecture, I will lecture how the growth units are incorporated into the crystal lattice for beginners of crystal growth. You will find the fundamental process of crystal growth -the step dynamics- and how the rate of crystal growth depends on the driving force of crystallization.

6(Tue.)14:00

Masaru Tachibana

Yokohama City University

Perfection of protein crystals by X-ray diffraction

X-ray topography is a non-destructive technique for imaging microscopic structural defects in nearly perfect crystals. It has been applied to a large variety of inorganic and organic materials and undoubtedly has played a major role in the search of defect-free crystals for the semiconductor industry. In my lecture, it is shown that X-ray topography can be a valuable tool in the study and understanding of protein crystal growth and diffraction properties. Recent report on the first observation of dynamical diffraction in protein crystals, which has been observed only in perfect crystals such as Si crystals, is also shown in the lecture.

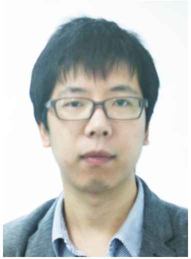
6(Tue.)14:40

Matthias Konrad-Schmolke

University of Gothenburg

Reactive fluid fluxes through solid rocks – constraints on mechanisms and element transport

Reactive fluids are interacting with crystalline rocks at every depth in the Earth's lithosphere. This fluid-rock interaction induces mineral reactions with implications ranging from nutrient transport for plants to element exchange between mantle and atmosphere in subduction zones. Furthermore, fluid-rock interactions influence the rocks' shear strength thus playing a fundamental role in the earthquake cycle. I will present several examples from subduction zone rocks that excellently preserve information about the mechanisms of fluid migration and fluid-mediated mineral dissolution and re-precipitation reactions. Such knowledge is crucial for the quantification of global scale element fluxes, but also for the understanding of fluid migration in subduction zones.



Zhisen Zhang

Xiamen University

Ice nucleation in hydrogel matrix

Water freezing remains a perennial topic of great relevance to many important aspects of our lives. One of unsolved puzzles of freezing is the question of how cooled of the idea pure water can withstand before freezing to ice. Commonly, -40 °C is regarded as the homogeneous nucleation temperature. However, previous work of our group has proved that water freezing is affected by dust particles even at a temperature as low as -40 °C. Here we report a new finding of water freezing water in hydrogel, in which the dust particles were embedded by the gelation process. And hence, the heterogeneous nucleation effect by the dust particles can be minimized. The observed effective nucleation temperature of ice in the hydrogel is -50 °C, suggesting that, instead of -40 °C, the homogeneous nucleation temperature of pure water could be lower than -50 °C.

6(Tue.)16:20

Gen Sazaki

Hokkaido University

The surface melting of ice crystals

We are studying thin water films, so called quasi-liquid layers (QLLs), that cover ice crystal surfaces at subzero temperature. Using laser confocal microscopy combined with differential interference contrast microscopy (LCM-DIM), we so far revealed that there exist two types of QLLs with different morphologies: a droplet type and a thin-layer type. In the symposium, we will show that the existence of such two types of QLLs can be explained by the transition of the wetting state of QLLs on ice surfaces. We found that such QLLs are kinetically formed as a metastable phase. We will also show the uptake of HCl in ice crystals: this triggers the ozone depletion.

6(Tue.)17:20

Katsuo Tsukamoto

Tohoku University/Osaka University

Optical in-situ observation of crystal growth interfaces

Mineral surfaces reflect the history how fast and where the crystals grew because these are closely related to the crystal growth mechanism. So as to understand the relationship, we have been using varieties of in-situ observations of crystal surface and the environments in various environments at low temperature to high temperature as high as 2000 K. The molecular-scale observation of crystal surface has been realized by using various techniques, AFM, STM and also phase-sensitive optical microscopy and interferometry. We show some examples how the growth history of minerals and crystals have been analyzed based on the knowledge of crystal growth mechanism.

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ST: Selected Topics
L: Lectures
Short oral (10 min.)

ime	3 SAT	4 SUN	5 MON	6 TUE	7 WED
8:00		ST J.M. García-Ruiz ST T. Sugiyama	ST H. Ohmoto ST N. Ozaki	ST X.Y. Liu L M. Konrad-Schmolke	Open Discussions, Awards Talks from Poster Presenters and Closing
9:00		Break ST K. Kakimoto	Break ST C.R. Li	Break L T. Okutsu	
10:00	Registration	Break ST E. Vlieg	ST A.P. Tsai	Break L S. Uda	
11:00		ST T. Fukuma	Lunch Banquet	L H. Miura	Excursion to Mt. Zao or Matsushima (1,500JPY/person, Max. 40 people) Arrive at Sendai Station at 17:00
12:00		Lunch		Lunch	
13:00	Opening K. Tsukamoto E. Vlieg				
14:00	H. Ohmoto Break T. Hibiya	ST T. Mizoguchi ST Q.S. Liu		ST M. Wang L M. Tachibana	
15:00	M. Maruyama M. Wang	Break L T. Ujihara	L M. Nakamura L E. Yokoyama	Break L Z. Zhang	
16:00	J. Sunagawa Break ST J. De Yoreo	L N. Akutsu	Break L Y. Kimura	L G. Sazaki	
17:00	ST G.W. Lee	Break L H. Imai	L J. Yamanaka	Break L K. Tsukamoto	
18:00	Dinner	Dinner	Dinner	Dinner	
19:00					
20:00	M. Maruyama Poster + *Practices of machine learning* *N. Akutsu*	S. Dalvi Poster + *Practices of machine learning* *N. Akutsu*	L.C. Chuang Poster	Poster report for students	
21:00					
22:00					

As of 23 Oct.. 2018