Grain alignment in protoplanetary disks

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Recently, ALMA has so far been revealed polarimetric properties of protoplanetary disks in (sub-)millimeter wavelengths. However, the origin of polarized light in these wavelengths is still controversial. In order to understand how polarized light is produced in these wavelengths, we apply the theory of radiative torque (RAT) alignment for studying protoplanetary disks around a T-Tauri star and perform 3D radiative transfer calculations to provide the expected maps of polarized radiation to be compared with observations, such as with ALMA. We revisit the issue of grain alignment for large grains expected in the protoplanetary disks and find that mm-sized grains at midplane do not align with magnetic field as the Larmor precession timescale for such large grains becomes longer than the gaseous damping timescale. Hence, for these grains the RAT theory predicts that the alignment axis is determined by the grain precession with respect to the radiative flux. As a result, we expect that the polarization will be in the azimuthal direction for a face-on disk. It is also shown that if dust grains have superparamagnetic inclusions, magnetic field alignment is possible for (sub-)micron grains at the surface layer of disks, and this can be tested by mid-infrared polarimetric observations.

Keywords: Protoplanetary disks, polarimetric observations, grain alignment

3D radiation hydrodynamics simulations of gravito-turbulence in protoplanetary disks

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Angular momentum transport in protoplanetary disks controls their time evolution and thus strongly affects the planet formation process within them. In some cold and massive protoplanetary disks, angular momentum can be transported by shear stresses associated with the gravitational instability (GI). A natural consequence of the long-range nature of gravity is formation of spiral arms as a result of GI, which globally transport angular momentum. On the other hand, Gammie (2001) showed another nonlinear outcome of GI, called gravito-turbulence, in which angular momentum transport can be described locally as in the alpha disk model (Shakura & Sunyaev 1973). Following Gammie (2001), many authors have studied numerically various aspects of the gravito-turbulence, but, in most cases, a simple cooling function with a constant cooling time has been used as in Gammie (2001).

In this paper, we present 3D radiation hydrodynamics simulations in a local shearing box to explore the outcome of self-gravity in a protoplanetary disk with realistic thermodynamics. We found that gravito-turbulence is sustained for a finite range of the surface density, from 20 to 50 times the one in the minimum mass solar nebula at 50AU, when the grazing angle of the irradiation is 0.02. The flow is laminar below the range while fragmentation occurs above the range. In the range of gravito-turbulence, the Toomre parameter decreases monotonically from 1 to 0.7 as the surface density increases while an effective cooling time takes an almost constant value that depends on the radius. The turbulent motions are supersonic at all heights, which dissipates through both shock waves and compressional heating. The compressional motions, occurring near the midplane, create upward flows, which not only contribute to supporting the disk but also to transporting the dissipated energy to the disk surfaces. We also show that the simple cooling function with a constant cooling time does not approximate the realistic cooling.

Keywords: protoplanetary disk, gravitational instability, turbulence

Synthesis of cosmic dust analogue particles in the newly developed ITP (induction thermal plasma) system

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Cosmic dust formed by condensation from high temperature gas around young and evolved stars or in the primordial solar nebula [1,2]. Some of them could be building block of our solar system.
The ITP (Induction Thermal Plasma) system enables the formation of nanoparticles from supersaturated vapors by homogeneous nucleation and growth because it offers vaporization of refractory materials at thousands of degree Celsius and very rapid quenching rates [3]. It can also control the evaporation and condensation environments by adjusting the characteristic of the thermal plasma. Moreover, condensation experiments from gases with various chemical compositions can be relatively easily performed in the ITP system because almost any reagents can be introduced into the plasma. For example, GEMS-like materials were reproduced in the different ITP system in the previous study [2].
In order to examine the formation processes of various cosmic dust analogues, a new ITP system (JEOL TP-40020NPS, max. 6 kW) was set up in our laboratory. The objective of the research is examination of the performance of the newly developed ITP system on production of nano-sized condensates simulating cosmic dust formation in circumstellar environments. We have already performed preliminary examinations using starting materials of SiO_2 (quartz), MgO (periclase), and Si-Mg-Fe-Na-Al-Ca-Ni-O in our ITP system [4]. In this study, we performed condensation experiments in the system of MgO-SiO_2 and examined the performance of the ITP system by changing plasma conditions.
We used mixtures of periclase and quartz powders with 1:1 molar ratio as stating materials for all experiments. The various operating parameters were applied to improve the evaporation rate and condensation conditions, such as feeding rates of starting material, reactor pressures, the presence of an additional slit gas, and the injecting direction of plasma forming gas. Plasma input power was fixed at 6 kW. The produced powders were analyzed by XRD, FT-IR, SEM, and TEM. Nano-sized condensates of amorphous silicate, forsterite, and protoenstatite were observed in most of the experimental products. We found that (1) the feeding rate of the starting material and reactor pressure control the vapor density and residence time at the high temperature regions of the plasma flame, (2) the vapor condenses into particles more rapidly by injecting the slit gas into the plasma flame, and (3) the injecting direction of the plasma forming gas changes temperature distribution of the plasma flame, which most influences condensation conditions. The plasma forming gas flows into the plasma generating torch axially (tangential flow) or swirly (radial flow). The radial flow provides a longer and narrower plasma flame that improves the residence time of the starting material at the high temperature region than the tangential flow. The more uniform nanoparticles were produced in the radial flow condition.

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Keywords: Cosmic dust, GEMS, Induction thermal plasma, Condensation experiment, Nanomaterial synthesis, Infrared spectrum

Condensation experiments in the Mg-Si-O system for understanding of circumstellar dust formation: dependence on the Mg/Si ratio.

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Silicates are major dust species around young and evolved stars, and in the interstellar medium. Experimental and theoretical studies on solid formation are crucial for understanding the origin of precursor materials of chondrites and dust formation around stars. Condensation experiments of silicates were performed in various systems, where most of the studies evaporated starting materials with compositions of $(Mg_x, Fe_{1-x})_2SiO_4$, SiO_2, and MgO [1-7]. Condensation from vapors with different Mg/Si ratio, however, has not been studied systematically. In this study, we performed condensation experiments of silicates from vapors with various Mg/Si ratios to examine the condensation sequence in different circumstellar environments.

Condensation experiments were carried out in a vacuum chamber. We produced Mg-Si-O gases by evaporation of (1) melts with Mg/Si~1 (Exp02 and 03) and (2) SiO_2 and MgO powders separately filled in Knudsen cells (Exp04-06) placed on the bottom of the crucible of 90 mm in depth. Here, the Mg/Si ratio was controlled by changing the size of the hole on the rids of the Knudsen cells to be 0.9, 1.6, and 20.0, respectively. The vapors condense onto Pt (Exp02-05) and Ir (Exp06) wires of 50-80 mm in length hung from the top of the crucible. The temperature gradient on the wire was measured by thermocouples before the experiments.

A mixture of SiO_2 and MgO powders were heated as a gas source at 1650 (Exp02) and 1580˚C (Exp03), which are higher than the melting temperature. We obtained condensates on the Pt-wires. In Exp02, forsterite was obtained at ~1570˚C and clino-enstatite at lower temperature regions. In Exp03, ortho- (or proto-) enstatite was observed at the highest temperature region (~1520˚C) and forsterite was not confirmed. Clino-enstatite covered the Pt-wire at lower temperatures than 1510˚C.

Quartz and periclase powders were put into Ir Knudsen cells separately and heated at 1580˚C (Exp03-06). No condensate was observed at >1360˚C. Forsterite covered the wires at <1350˚C and enstatite was not condensed at lower temperatures. No clear difference was observed between the three experiments with different Mg/Si ratio of 0.9-20.0.

Fractional evaporation may have occurred from Mg-Si-O melts, and the gas composition gradually enriched in Si compared to Mg during the experiments. We did not use Knudsen cells for the experiments Exp02 and 03. Therefore, the differences between the condensation experiments from gases evaporated from melts and powders may be the Mg/Si ratio and gas fluxes. As future works, we plan to perform experiments with much lower Mg/Si ratios and with higher gas fluxes (higher supersaturation ratios) to determine the condition to form clino- and proto-enstatite from gas phases.

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Keywords: condensation, experiments, silicate, circumstellar dust

Evolution of molecules in space: from interstellar clouds to proto-planetary nebula

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Our understanding of the origin and evolution of planetary systems has been mostly limited to the dynamics. The importance of chemistry has been emphasized, however, systematic studies about chemical evolution have not yet been performed. We have thus started research project on “Evolution of molecules in space” supported by Grant-in-Aid for Scientific Research on Innovative Areas from MEXT, Japan from 2013.
We focus our attention on the most abundant solid materials in space: ices and organic materials. How do these molecules evolve in space? We aim at answering this question by interdisciplinary approaches including laboratory and theoretical studies about surface processes, observation of young stellar objects, modeling of molecular cloud and protoplanetary-disk chemistry, and analyses of extraterrestrial materials.

We are now investigating the evolution of molecules by following groups; (1) Experimental studies about surface reactions of atoms and molecules and photochemical reactions of solids at low temperatures to mimic phenomena occurring in molecular clouds (PI: A. Kouchi, Hokkaido Univ.), (2) Heating experiments of molecular-cloud organics and Fischer-Tropsh type surface reaction experiments to mimic phenomena occurring in proto-planetary nebulae (PI: H. Nagahara, Univ. of Tokyo), (3) Observation of young stellar objects by radio telescopes (ALMA, ASTE etc.) to understand the evolution and variety of organic molecules (PI: S. Yamamoto Univ. of Tokyo), (4) Modeling of surface processes and developing of chemical network model (PI: T. Fukazawa, Meiji Univ.), and (5) Analyses of chemical and isotopic composition of organic molecules in meteorites and cometary dust (PI: H. Yurimoto, Hokkaido Univ.). I will introduce some important achievements of respective groups.

Our project will contribute to not only the understanding of origin and evolution of molecules in space but also the analysis of returned samples by Hayabusa 2 and OSIRIS-REx. We have developed some new analytical setups: High-resolution imaging-type soft X-ray microscope/spectrometer, two-dimensional HPLC-MS for amino acids analysis, high-sensitive HPLC-MS for organic material analysis, etc.

Keywords: Evolution of molecules, Ices, Organic materials, Interstellar molecular clouds, Proto-planetary disk

Reproducing interstellar infrared spectrum by modeling a hydrocarbon pentagon-hexagon combined molecule

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Interstellar infrared spectrum coming from polycyclic hydrocarbon molecules shows a ubiquitous pattern in a wavelength of 3-15 micrometer (1). These years, thousand kind of molecules were test and discussed as a candidate. However, any convincing single molecule was not discovered by both experiment and calculation. Here, promising single molecule was studied by quantum-chemistry first principles calculation focusing on hydrocarbon pentagon-hexagon combined molecule parametarizing charge and spin state. Among many candidates, better one was dication (C23H12)+2 having two pentagons and five hexagons (2). Calculated main peaks were 3.2 , 6.4, 7.6, 7.8, 8.6, 11.2, 12.7 and 14.1 micrometer. Those show very good coincidence with astronomically observed values as 3.3, 6.2, 7.6, 7.8, 8.6, 11.2, 12.7, and 14.3 micrometer. Also, another small molecule (C12H8)3+ having one pentagon and two hexagons shows good coincidence at major wavelength of 3.2, 6.4, 7.5, 7.8, and 11.2 micrometer. This is the first case to give good coincidence by a single molecule. References: (1)Christiaan Boersma et al, Astrophysical Journal 690.1208(2009) (2)Norio Ota, arXiv:1402.0009(2014) (3)Norio Ota, arXiv:1510.07403(2015)

Keywords: interstellar dust, infrared spectrum, PAH

Detections of Long Carbon Chains CH_3CCCCH, C_6H, *linear*-C_6H_2 and C_7H in the Low-Mass Star Forming Region L1527

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A richness of long carbon chains in the warm carbon chain chemistry (WCCC) region has been searched in the 42-44 GHz region by using Green Bank 100 m telescope. Long carbon chains C_7H, C_6H, CH_3C_4H, and *linear*-C_6H_2 and cyclic species C_3H and C_3H_2O have been detected in the low-mass star forming region L1527, performing the WCCC. The detection of C_7H is for the first time in molecular clouds. While the abundance ratios of carbon chains in between L1527 and the starless dark cloud Taurus Molecular Cloud-1 Cyanopolyyne Peak (TMC-1 CP) have a trend of decrease by extension of carbon-chain length, column densities of CH_3C_4H and C_6H are on the trend. However, the column densities of *linear*-C_6H_2, and C_7H are as abundant as those of TMC-1 CP in spite of long carbon chain, i.e., they are not on the trend. The abundances of *linear*-C_6H_2 and C_7H show that L1527 is rich for long carbon chains as well as TMC-1 CP.

Keywords: carbon chain, radio, molecular cloud

Reaction efficiency between hydrogen and carbon monoxide on a catalytic substrate of iron, nickel or its alloy

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Reaction of hydrogen and carbon monoxide on a catalytic substrate to form methane and water has widely been used to synthesize fuel and called the Fischer-Tropsch reaction (FT reaction). Typical conditions of the FT reaction for manufacturing application is a total gas pressure of 10^5-10^6 Pa with a ratio of H_2 / CO = 2 at 500-650 K together with a catalysis of Fe, Co or Ru[1]. Then, water-gas shift reaction has been occurred as a side reaction; carbon dioxide and hydrogen molecules form from carbon monoxide and water. The efficiencies of both reactions depend on the substrate, temperature, pressure and other conditions. Cobalt has most been used as a catalysis because of the lower activity of the side reaction [2,3]. Although the FT reaction has been used for long years, the atomic/molecular scale mechanisms that govern the FT reaction are still disputable [4]. Therefore, it is not obvious that the results of the reaction experiments are able to extrapolate to the actual solar nebula environment. Here we demonstrate the reaction rates in the solar nebula conditions (below 500 K and under 10^2 Pa) on the surface of cosmic dust particles, such as iron, iron-nickel alloys and nickel.
We developed an experimental system to test the catalytic chemical reactions in the temperature and pressure ranges of 50-800 K and 10^{-3}-10^3 Pa, respectively, using a metallic plate as a catalytic substrate. Our experimental system has a temperature-controlled substrate, a Fourier transform infrared spectrometer (FT-IR), and two quadrupole mass spectrometers (Q-MSs). FT-IR is able to measure the vibration modes of adsorbed and produced molecules on the substrate. Currently, several IR features has been detected at the temperature below 150 K. To identify the mass signal of produced methane and water in the Q-MSs spectra, deuterium was used instead of hydrogen. The intensity of the signal of masses 20 and 44 decreases as temperature decrease from 800 K. The mass 20 corresponding to D_2O and CD_4, which are first products in the Fischer-Tropsch type reaction, was detected. Simultaneously, mass 44 corresponding to CO_2 was also detected. In our presentation, the substrate dependence of the reaction efficiency will be presented.

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Keywords: Fischer-Tropsch reaction, Surface reaction, Solar nebula

New formation mechanisms of meteoritic amino acids based on the discovery of hydroxy amino acids identified in the Murchison meteorite

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ntroduction: Carbonaceous chondrites contain a diverse suite of extraterrestrial amino acids, which have various structures such as α, β, γ or δ amino-group [1], while terrestrial life use only α-amino acids. The distribution of meteoritic amino acids had been influenced by aqueous alteration on the meteorite parent body (e.g. α-aminoisobutyric acid versus β-alanine [2], and L-enantiomeric excess of isovaline [3]). However, a comprehensive formation mechanism, which could explain the diversity of meteoritic amino acids, remains unclear. In our previous study, nine new hydroxy amino acids and one β-aminodicarboxylic acid were identified in the extract of the Murchison for the first time (Koga and Naraoka, under revision). In this study, the simulation experiments of amino acid synthesis were performed under plausible conditions of the meteorite parent body in order to pursue their formation mechanisms.

Materials and Methods: The aqueous solutions containing ammonia/formaldehyde/acetaldehyde and/or glycolaldehyde (100/10/1/1 by mol) with NH_3/H_2O (1/100 by mol) were heated at 60 ˚C for 6 days in a N_2-purged glass ampoule with or without olivine or quartz powder with the water/mineral ratio of 1/9 (by weight). The reaction mixtures were extracted with hot water at 100 ˚C for 20 h. The supernatants were divided into three fractions: one hydrolyzed with 6M HCl for analysis of amino acid distribution, and two non-hydrolyzed for investigation of their precursors. The hydrolyzed and one non-hydrolyzed fractions were analyzed by GC/MS with a Chirasil-L-Val capillary column. The other non-hydrolyzed fraction was analyzed by GC/MS with a DB-5 capillary column.

Results and Discussion: The simulation experiments gave totally 20 amino acids including the nine new amino acids identified in the Murchison extract by our previous study (Koga and Naraoka, under revision). Glycine was the most abundant (approximately 0.1 % relative to the total initial carbon concentration of aldehydes), which is the similar occurrence as observed by the previous study. The amount and variety of amino acids increased in the presence of olivine compared to those in the absence of olivine and the presence of quartz. When glycolaldehyde was used in addition to formaldehyde, acetaldehyde and ammonia, the yield of hydroxy amino acids increased 1.4 times, but β-aminodicarboxylic acid decreased by one-fifth relative to the experiment in the absence of glycolaldehyde. These results indicate that formose reaction with ammonia in the presence of mineral is an important formation pathway to produce meteoritic amino acids during aqueous alteration on the meteorite parent body. In addition, the identification of a hydroxy amino acid precursor (3-Hydroxy-2-pyrrolidinone) is suggestive of a possible formation pathway using the formose reaction products with ammonia.

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Keywords: Carbonaceous chondrite, Amino acid, Formose reaction, Aqueous alteration, Meteorite parent body

Estimation of surface composition of asteroids in combination with Bus-DeMeo taxonomy and other physical observations

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The classification of asteroid’ s surface was done using the wavelength of visible light (eg, Tholen 1984, PhD thesis, Univ. Arizona; Bus & Binzel 2002, Icarus 158, 146), but due to the development of infrared observation technology in recent years, a method which extended to near infrared in addition to visible light has been proposed (DeMeo et al. 2009, Icarus 202, 160). By expanding the range of adaptation up to near infrared, in particular, those that were feature-less with visible light became clearly classifiable. Physical observations of asteroids are carried out also other than visible/near infrared spectroscopic observation. By adding the Bus-DeMeo classification method and other physical observation result information, it is thought that physical information of the asteroid surface layer can be extracted. It is the purpose of this research to derive new constraints on the composition of asteroids in the asteroid zone by combination of information.

Keywords: asteroid, meteorite

H^+ irradiation experiments to pyroxene and olivine for simulating space weathering by solar wind.

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The space weathering observed on the surface of asteroids is caused by micrometeorite bombardment, solar wind irradiation, and cosmic ray irradiation [1-3]. From the analysis of the regolith particles that Hayabusa spacecraft recovered from an S-type asteroid, 25143 Itokawa, the evidences of the space weathering on Itokawa, such as vesicle structures (blisters) and amorphous layers (space-weathered rims), have been confirmed [4-6]. It has been proposed that the blisters and space-weathered rims might have been formed mainly through solar wind irradiation rather than by micrometeorite bombardment [4].
Solar wind consists of 1 keV H^+ ions (95.41 %) and 4 keV He^+ ions (4.57 %) [7]. Irradiation experiments of 1 keV H^+ ions and 4keV He^+ ions to minerals consisting of the Itokawa regolith are important in order to evaluate the influence of solar-wind irradiation on formation of the blisters and space-weathered rims on the Itokawa regolith. Many irradiation experiments of 4 keV He^+ ions have been already performed, but the irradiation experiment of 1 keV H^+ ions has been hardly carried out [e.g., 8].
In this study, we examined the performance of the ion-irradiation equipment under development in ISAS/JAXA and then performed the irradiation experiments of 1 keV H^+ to orthoenstatite and olivine with different compositions, which are the major minerals consistent of ordinary chondrites.
We measured the shape and size of the ion beam by moving the one-dimensional multipoint Faraday cup. The half maximum full-width of the ion was 1.2-2.7 mm and the current density was 0.52-1.22 μm/cm^2. We verified the stability of the ion beam at least for ten hours. The confirmed performance of the ion irradiation system enables the 1 keV H^+ irradiation with a dose of at least 10^{17} ions/cm^2.
As targets of irradiation experiments, we prepared rectangular samples of orthoenstatite (En_{99}, Tanzania), forsterite (Fo_{100}, synthetsis), and olivine (Fo_{92}, San Carlos). The sample size is 3 mm x 5 mm x 0.5 mm. We mechanically polished the samples (until 0.25 μm roughness) and performed the chemical polishing with colloidal silica to remove the damage layer of the surface. Finally, the surfaces of samples were cleaned by the ultrasonic cleaning. The irradiated samples were observed with an FE-SEM (JEOL JSM 7001F).
FIB-lift-out sections were prepared with FE-FIB (FEI Helios NanoLab 3G CX) and observed with FE-TEM (JEOL JEM 2100F).
On the surface of the irradiated enstatite (10^{17} ions/cm^2), an amorphous layer (26 nm) was observed. The thickness of the amorphous layer is consistent with the width of the damage layer promoted by 1keV H^+ irradiation calculated with the SRIM [9]. However, amorphous layer was also observed in the unirradiated area, which indicates that the damage due to the mechanical polishing in the sample preparation had not been removed by the chemical polishing. The blisters of 30 nm in diameter and $3x10^{10}$ cm^{-2} in density, and the sharper boundary of amorphous layer were observed only in the irradiated area. Compared with the Itokawa particles [4-6], the irradiated enstatite sample and Itokawa particles show similar size, density, and formation depth of the blisters, although the thickness of the amorphous layer of the irradiated enstatite (26 nm) is less than Itokawa enstatite particles (40-50 nm). The thicker amorphous layers on the Itokawa particles are due to deeper implantation depth of 4 keV He^+ than 1 keV H^+ [4,9]. These results suggest that the blisters on the surface of Itokawa particles were mainly formed by 1 keV H^+ ion

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Keywords: space weathering, solar wind

Adsorption process of ion on amorphous ice surface

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In interstellar molecular clouds, various molecules (for instance, H_2O, NH_3, CO, CO_2, and so on) are formed from elements such as H, C, O, and N [1]. Most of H_2O exists as a thin shell of amorphous ice around dust grain. The molecules undergo chemical evolutions to organic molecules through various processes on the surface of amorphous ice [2]. Thus, the surface structure of amorphous ice is an important factor to understand the molecular evolution of organic molecules in molecular clouds. To investigate the effects of adsorption of ion on the surface structure of amorphous ice, the molecular dynamics (MD) calculations of amorphous ice with NO_3^- were performed.

The MD calculations were performed using an atom-atom potential model, KAWAMURA potential model [3]. The amorphous ice was prepared by quenching of a liquid phase consisting of 2760 water molecules from 280 to 235 K with 2.5 K/fs in cooling rate. After annealing at 235 K, the system was cooled to 10 K. The density of amorphous ice at 10 K was controlled with the time period of the annealing at 235 K. To equilibrate the fundamental cell, the MD code was run for 40 ps at 10 K. Then, an ion (NO_3^-) was put in a position, such the center of nitrogen in ion was at a distance of 0.5 nm from the outermost hydrogen atom in surface. An infinite surface was simulated by replicating the cell in the directions parallel to the surface using periodic boundary conditions. The pressure was kept at 0.1 MPa. The layer with 0.5 nm in thickness from the outmost atom was analyzed as the surface layer.

The result shows that the atomic displacement parameters (ADP) of oxygen and hydrogen of water molecules in surface layer increase during the adsorption of NO_3^-. The values are diminished with formation of hydrogen bonds with surrounding water molecules, and gradually approach the values of pure amorphous ice without ions. For surface with NO_3^-, three oxygen atoms of NO_3^- form hydrogen bonds with hydrogen atoms in dangling bonds of water on the surface layer. When an ion is adsorbed, surrounding water molecules rotate to form hydrogen bonds with the ion. Thus, the rearrangement of water molecules occur even at low temperature. The result indicates that the thermal vibrations of water molecules are enhanced with adsorption and diffusion of ions on the surface. To investigate the effects of ion adsorption on smoothing of surface roughness, the potential map of surface layer were calculated. The results show that the potential map charges with a collision of ion on a convex position, whereas no charge was observed when the ion adsorbs on a concave position. This indicates that the smoothing of surface roughness of amorphous ice at low temperature results from ion collisions. The effects of ion adsorption might have important implications for surface reaction in interstellar molecular clouds.

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Surface Structures of Forsterite Crystal and Glass

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In interstellar molecular clouds, elements such as hydrogen, oxygen, carbon, and nitrogen deposit on dust grains, and form various molecules (e.g., H_2O, CO, CO_2, NH_3, CH_4, H_2CO, CH_3OH, and so on). These molecules undergo chemical evolutions to organic molecules through various processes on the surface of dust grains [1]. Forsterite (Mg_2SiO_4) and enstatite ($MgSiO_3$) have been observed in interstellar molecular clouds and young stellar objects [2]. Although various studies have been performed for bulk structures of forsterite and enstatite, their surface structures are less conclusive [3]. To investigate the surface structures of forsterite in crystalline and glassy states, molecular dynamics (MD) calculations were performed. The surface structure is one of the important factors governing the chemical evolutions in interstellar molecular clouds.

The MD calculations were performed using an atom-atom potential model [4]. The potential parameters were empirically determined by constraining the model to reproduce the experimental results of density, thermal expansion coefficient, and bulk modulus [4]. The glass structure was prepared by quenching the liquid phase consisting of 2400 Mg_2SiO_4 from 3000 K to 10–1750 K with 2 K/fs in rate. An infinite surface was simulated by replicating the cell in the directions parallel to the surface using periodic boundary conditions. The pressure was kept at 0.1 MPa. The MD code was run with NTV ensemble at each temperature for 500 ps with a time step of 0.5 fs. The layer with 0.5 nm in thickness from the outmost atom was analyzed as the surface layer.

The result shows that the melting temperature of forsterite crystal with surface layer was 1927 K. This value is lower than the MD result of bulk state without surface (2418 K [4]) and experimental result (2171 K [5]). This depression of the melting temperature is attributed to the structure and thermal vibrations of atoms in surface layer of forsterite crystal. The nearest Si–Si distance, which was analyzed using the pair correlation functions of atoms, for surface layer of crystal is larger than that of internal part. Furthermore, the amplitudes of thermal vibrations of atoms in surface layer are larger than those of internal part. The results indicate that a surface layer with low density and high thermal vibrations exists in forsterite crystal. The amplitudes of thermal vibrations in surface layer increase with warming and approach the values of the bulk state at its melting point (i.e., 2418 K) at around 1927 K. This induces the depression of the melting temperature for system with the surface layer. For glassy state, a surface layer with short Si–Si distance exists, although the amplitudes of thermal vibrations of atoms are large in comparison with the values of the internal part. This inverted tendency may be resulted from an inhomogeneous structure of surface layer in the glassy state. The surface structures of crystalline and glassy forsterites have important implications for adsorption, diffusion, and chemical reaction in interstellar dust grains.

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Keywords: Forsterite, Surface, Interstellar molecular clouds, Molecular dynamics

N-heterocyclic compound synthesis from aldehydes and ketone with ammonia: A simulation of organic reactions on the meteorite parent bodies

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[Introduction]
Carbonaceous chondrites have the most primitive chemical compositions in the solar system and contain volatile components such as water and carbon. In spite of their primitive character, most carbonaceous chondrites have had experienced aqueous alteration on parent bodies, which was revealed by the occurrence of hydrous minerals. The meteoritic carbon are present mainly as organic matter, in which soluble organic matter (SOM, ~1 to ~30 wt%) consists of relatively low-molecular-weight compounds such as carboxylic acids and amino acids. The rest major carbon exists as insoluble organic matter (IOM) having high-molecular complicated structures. Therefore, the aqueous alteration must have influenced the organic-mineral interactions. In order to study the chemical evolution of organic matter in the solar system, the role(s) of minerals should be clarified. In this study, we performed simulation experiments of organic compound synthesis using ammonia (NH_3), formaldehyde (HCHO), acetaldehyde (CH_3CHO), propionaldehyde (C_2H_5CHO) and acetone (CH_3COCH_3), which are simple molecules found in molecular clouds, under the aqueous environment in the presence or absence of minerals.
[Materials and Methods]
The several aqueous mixtures with various ratios (by mol) of NH_3 (1 to 10) /HCHO (0.1 to 1) /CH_3CHO (0.01 to 0.1) /C_2H_5CHO (0.01 to 0.1)/CH_3COCH_3(0.01 to 0.1) were heated in the presence of powdered mineral including forsterite (San Carlos), magnetite (Utah), synthetic forsterite or amorphous silicate (Mg_2SiO_4 in composition) at 60 to 80℃ for 144 to 192 hours in N2-purged glass ampoules. A total of 20 runs of simulation experiments were performed. The reaction product was extracted with methylene chloride/methanol (2/1, by volume) and analyzed by high performance liquid chromatography/mass spectrometery.
[Results and Discussion]
Many compounds were observed at the range of m/z 100-400 in all reaction products. Of the identified compounds, alkylpyridines ($C_nH_{2n-5}N$), alkylimidazoles ($C_nH_{2n-3}N_2$) and hexamethylenetetramine ($C_6H_{12}N_4$, HMT) were the main products for each run. The compounds that have not been identified but represented by compositional having $C_nH_{2n-1}N_3O$ in composition were also identified as a main product. Although alkylpyridines and alkylimidazoles have been detected from carbonaceous chondrites (e.g. Yamashita and Naraoka, 2014). Although HMT has been reported as a main product during interstellar analog experiment by UV irradiation at low temperature (Vinogradoff et al., 2011), HMT has not been found in meteorites. HMT is relatively abundant in the products with the absence of minerals. However, the HMT amount decreased in the presence of the amorphous silicate and forsterite (San Carlos), instead of increasing production of alkylpyridines and alkylimidazoles. The minerals could control the reaction pathways as a catalyst. In particular, as amorphous silicate is the main solid phase in the interstellar environments (F. Kemper etal., 2004), it may have important roles for the evolution of extraterrestrial organic matter. Further experiments are needed to identify the intermediate compounds as well as to observe the change in mineral phases during the reactions.

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Keywords: Chemical Evolution, Mineral-organic interaction, Aqueous alterlation, N-Containing Compound, Carbonaceous chondrite

Meteoritic organic compound analysis by nano-liquid chromatography/mass spectrometry

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[Introduction]
Carbonaceous chondrites, which have the primitive chemical composition in the solar system, contain volatile materials including water and organic matter. Since biologically-relevant molecules such as amino acids, nucleobases were detected in meteorites(e.g. Burton et al., 2012), meteoritic organic matter has been investigated with respect to the origin of life. So far the organic compounds have been generally analyzed using the powder sample of sub-g to g meteorite with solvent extraction followed by chromatography. The powdered sample has lost its location information such as mineral textures, even though the primitive meteorites have heterogeneous composition in chemistry and mineralogy. Since most carbonaceous chondrites experienced aqueous alteration on the parent bodies, the understandig of mineral associaton with organic compounds is necessary to reveal chemical evolution in extraterrestrial environments. Futhermore, non-destructive organic analysis is preferred especially for precious samples. In this study, we will develop an analytical method of organic compounds using an intact micro-meter sized grain of extraterrestirial meterial with high-sensitive nano-liquid chromatography (nanoLC) coupled with high-resolution mass spectrometry(HRMS).
[Materials and Methods]
A single grain (~300 to 900 μm) was obtained by chipping from carbonaceous chondrites (Murchison and Murray; CM2). Each grain (0.168-2.392mg) was soaked in 5.0 μL of methanol(MeOH) followed by sonication or mixing. One micro-litter of each extract was subjected to nanoLC/HRMS ($m/\Delta m$=~140,000 at m/z 200) with electrospray ionization (positive ion) using C18 reversed phase column or amide column. The eluent solvents were mixture of acetonitrile, water and formic acid. All analytical procedures were performed in a clean room.
[Results and Discussion]
Apparent changes were not observed on the grain surface before and after the analysis. Many alkylated homologous CHN and CHNO compounds were distinguished by every 14.0156 (m/z; -CH_2-) and peaks shift in the retention time of mass chromatogram. The occurence of homologous series is consistent with previous studies (Schmitt-Kopplin et al., 2010; Yamashita and Naraoka, 2014), suggesting the carbon-chain elongation by stepwise reactions from small molecules. The homologous series of $C_nH_{2n-5}N$(n=5-26), C_nH_{2n-7N}(n=9-28), $C_nH_{2n-1}N_2$(n=5-23), $C_nH_{2n-1}NO$(n=3-20), $C_nH_{2n-3}NO$(n=9-12) and $C_nH_{2n-5}NO$(n=6-26) were detected from the Murray meteorite. In contrast, the only series of $C_nH_{2n-5}N$(n=5-24) and $C_nH_{2n-7}N$(n=10-26) homologous series were detected in Murchison meteorite. The range of carbon number in the homologous series varied depending on the meteorites, whch may imply heterogeneity of organic compounds in the meteorites. Such a heterogeneous distribution may be associated with the mineral occurance. The fluid flow on the parent body may also affect the compound distribution by the (geo)chromatographic effect. Further investigations are needed to clarify the relationship between the meteoritic texture and the distribution of organic compounds.

Keywords: organic compound, carbonaceous chondrite, nanoLC/HRMS, heterogeneity

Isotopic Analysis of Presolar SiC Grains with the Post-Ionization SNMS

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For unveiling nucleosynthesis during stellar evolution, in-situ isotopic analyses of individual presolar grains have played important roles. So far, we have been developing a new mass spectrometer, Secondary Neutrals Mass Spectrometer (SNMS) with a femto-second laser, in order to enable further sensitive and higher mass/spatial-resolution measurements. At the conference, we' ll report our recent progress of development of SNMS and application to the analysis of SiC grains collected from Murchison meteorite. As preliminary results, we detected isotopic anomalies of major elements (Si and C), which is consistent with those of previous works. We will also refer the challenging isotopic measurements of other minor elements.

Keywords: Stellar Evolution, Presolar Grain, Isotopic Analysis

Formation of celestial body that was caused by the change of electronic states of matter

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Gravitational collapse of interstellar gas and condensation of cosmic dusts has been investigated [1]. But, electron-electron interactions increase by the increase of mass of celestial body. The change of electronic state increases bonding force. Large celestial body can become the core for gravitational collapse of hydrogen gas.
Coulomb force that binds neighboring atoms in vicinity of 10^{-10} m is about 10^{36} times powerful of gravitational force. Cold nanoparticles of interstellar medium can be clustered by the electron-electron interaction. Molecules of water contributed to growth of the cluster. The percentage of effect of short-range force on a cluster comprised of larger solid elements is decreased.
The gravity increases cumulatively with increase of mass regardless of the points of chemical bond. If planet becomes larger than 2.0×10^{9} kg, gravitational force of planet is more than short-range force. Large planetesimal captures small planetesimal by the gravity. Huge mass of celestial body can hold the hydrogen. Temperature of interior of planet become high by the gravitational potential energy.
Coulomb force and gravitational force work concurrently. Long period of growth is necessary in the early stages for the growth due to short-range force. While, gravitational collapse of interstellar gas is progressed in a short time due to existence of the gas of about 100 times mass of cosmic dust. The Sun is not the first generation of stars. The protostar of the Sun was growing before gravitational collapse of gas. There is metallic electronic state of hydrogen outside of core. The nuclear fusion begins at hydrogen layer. Radioactive substances contained in meteorite indicates that those were born from solid core by explosion due to nuclear fusion.
Please see more information at Website; “https://youtu.be/GMmvjU2CdKM”, “https://youtu.be/HwBjqYpDdu0”.

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Keywords: protostar, cosmic dust, intermolecular bond, short-range force, gravitational collapse, nuclear fusion

Mid-infrared observations of the dust-forming classical nova V2676 Oph with Subaru/COMICS

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A dust-forming nova V2676 Oph (discovered in Mar 2012) was the first nova to provide evidence of both C_2 and CN molecules during its near-maximum phase and evidence of CO molecules during its early decline phase (Nagashima et al. 2014). The derived carbon- and nitrogen-isotopic ratios in the nova (Kawakita et al. 2015) are consistent with that the nova explosion was hosted by a CO-rich white dwarf (WD) star. To confirm a type of the hosting WD (CO-rich or ONe-rich), we performed the mid-infrared imaging and low-resolution spectroscopic observations of V2676 Oph with COMICS mounted on the Subaru telescope in June 2013 and May 2014 (482 days and 782 days respectively after its discovery). No clear [Ne II] emission line at 12.8 micron was observed. Based on the absence of [Ne II] emission, the WD hosting V2676 Oph is considered a CO-rich WD. Both types of dust grain, carbon-rich and oxygen-rich, were detected on both dates, although this nova is considered as a Carbon-rich (C/O > 1) based on the presence of C_2 observed earlier. The 11.4 micron unidentified infrared emission was also detected on these dates. Non-equilibrium processes are likely to be responsible for the grain formation in the nova.

Keywords: nova, dust, infrared

Silicate dust evolution in protoplanetary disks

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Silicate is the dominant solid component in circumstellar environments. Infrared spectroscopic observations have shown that both crystalline and amorphous silicate dust are present in protoplanetary disks, and crystalline silicate dust seems more abundant in the inner warm region of the disks. This suggests that thermal annealing of interstellar amorphous silicate dust occurred in the disk and changed the dust properties of disk dust temporally and spatially with disk evolution. Some of those processes occurred in the early Solar System may have been recorded in fine-grained matrices of less altered/metamorphosed chondrites, which contain abundant amorphous silicates and a small fraction of presolar silicate grains. Laboratory experiments help us extract the record of disk thermal processes from natural samples quantitatively. We have done experiments on crystallization and hydration experiments of amorphous silicates and evaporation and condensation experiments of crystalline silicates, focusing on kinetics of these processes. In this presentation, based on experimentally-obtained kinetic data, we will discuss the silicate dust evolution in protoplanetary disks.

Keywords: silicate, protoplanetary disk, kinetics

