

Nucleation process from vapor due to molecular dynamics simulations: effect of the sticking probability

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In the previous studies (Tanaka et al. 2005, 2011), we performed molecular dynamics (MD) simulations of nucleation from vapor of Lennard-Jones (L-J) type molecules and found that the semi-phenomenological (SP) model reproduces very well the nucleation rates obtained from the MD simulations. In this study, we performed MD simulations of nucleation from vapor for systems of 4000 water molecules to test nucleation theories. Simulations were done for wide ranges of the initial supersaturation ratio ($S=4-400$) and temperature ($T=250-375$ K). Through comparison with the nucleation rates and the cluster size distributions obtained from our MD simulations, we investigated the validity of the SP model. Our results show that the semi-phenomenological model reproduces well the size distributions of the clusters and the nucleation rates. Furthermore, the sticking probability of vapor molecules onto clusters was examined in MD simulations, by observing the growth rate of stable clusters larger than the critical size. In all runs in the present study, the values of the sticking probability are larger than 0.1. Our results show that the obtained sticking probability depends on the supersaturation ratio.

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In-situ observation of nucleation process under microgravity by an aircraft

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To understand the formation process of cosmic dust particles with nm to sub-micrometer in size, dust analogues have been produced in the laboratory. The gas evaporation method has a similarity in the dust formation process in space, where dust forms by a condensation from gas phase via homogeneous nucleation in most case. Nucleation determines characters of dust, such as size, number and composition. However, nucleation process has been unknown not only in universe but also in the laboratory. Recently, we succeeded in directly observing the temperature and concentration during homogeneous nucleation in the vapor phase by interferometer under the gravity [1,2] To understand the homogeneous nucleation quantitatively, we applied nucleation theories to the experimental results and determined the following results: the surface free energy, the size of critical nuclei, determination of polymorph, fusion growth and sticking probability. In particular, surface free energy and sticking probability are most important parameters to know the characters of cosmic dust. Here, we will show the recent results in microgravity by using an aircraft. Microgravity experiment has an advantage to determine above mentioned values more certainly due to suppress the thermal convection, which generates inhomogeneous formation condition and secondary growth in the flow.

Smoke particles of WO_3 , SiO , Mn, Fe, Au or NaCl were produced in a specially designed smoke chamber setting with a Mach-Zehnder-type interferometer with two wavelengths lasers, which can obtain two unknown parameters simultaneously, i.e., concentration of evaporant and temperature.

When an evaporant is initiated in an inert gas, the evaporated vapor subsequently cools and condenses homogeneously in the gas atmosphere. Condensation temperature depends on surface energy and sticking probability. Both parameters can be determined from the condensation temperature and the size of produced particles, respectively.

In case of Mn and WO_3 , condensation occurred at 660 and 600 K below the equilibrium temperatures, and the degree of supersaturation was as high as 10^5 and 10^9 , respectively. The condensation temperature, number density, and size of particles for Mn experiment were consistent with the values calculated by the semi-phenomenological nucleation theory. On the other hand, however, the results have a gap with the values calculated by the nucleation theories in case of WO_3 and NaCl. One of the reasons may be due to secondary growth. Since there is strong thermal convection generated by the hot evaporation source in the chamber, condensed particles follow the convection and possibly grow in the way as gas cools. As the result, size and number density could be different from the theory. In the same reason, estimation of the sticking probability will be difficult. It has been expected that microgravity experiment gives us more certain results due to suppress the thermal convection.

Recently, we firstly performed the gas evaporation experiments in microgravity using the aircraft. Here, we will present the brief results and show the difference from gravity experiment. Since microgravity environment strongly suppresses the thermal convection, evaporated vapor diffused simply to the direction of centric distance and condensed at the wider area compared with gravity condition due to no convection. Then, it can be concluded that condensation in microgravity occurred farther from the evaporation source compared with gravity experiment. In case of microgravity experiment, since condensation and growth occur at the same place due to no convection, secondary growth is negligible and the results are able to compare with the nucleation theories. As the result, surface free energy and sticking parameter will be determined more certainly.

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[2] Y. Kimura, et al., J. Crystal Growth, 316 (2011) 196.

Keywords: Nucleation, dust, nanoparticle, in-situ observation

Thermal instability of gas-dust fluid system

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We carry out hydrodynamics linear stability analysis of 1-dimensional gas-dust fluid system. We focus on the thermal instability caused by the radiative cooling. If the cooling in a region takes place effectively, the gas temperature and the pressure decrease, and a flow converging to the region is driven. Then the dust particle number density in the region is enhanced by the gas drag force, and the cooling rate from the region can be raised as well because the cooling rate is proportional to the dust number density. This one-way process would lead to instability.

As an initial state, we assume that the system is static and the gas temperature is higher than the dust temperature. For retaining this state, we assume a hypothetical heat function for gas that is a function of the gas temperature and the gas density. As the cooling mechanism of the system, we suppose that the radiation from dust particle leaves the system without being absorbed again. Thermal energy is transferred between the gas and the dust particle by gas-dust collisions. At the same time the gas and the dust particles are dynamically coupled by drag force.

As a result of our linear analysis, we obtain a dispersion relation. We find that when a gas-temperature derivative and a gas-density derivative of the heat function satisfy certain criteria, an unstable mode emerges. When the instability takes place, the fluctuation of the dust particle number density grows.

Our result implies that if a realistic heat function meets the obtained criteria, a dust accumulation may occur in a protoplanetary disk. And this accumulation may lead to the planetesimal formation.

Keywords: hydrodynamics linear stability analysis, dust accumulation, chondrule formation, planetesimal formation

Cr-54 anomalies and accretion ages of meteorite parent bodies

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A positive correlation between ^{54}Cr excesses and accretion ages is observed among meteorites including iron meteorites, palasites, mesosiderites, aubrites, HED meteorites, angrites, ureilites, acapulcoites and chondrites (including E, O, R, CK, CO, CV, CH-CB, CR, CM and CI) [1]. This suggests that ^{54}Cr carriers were injected into the forming solar nebula. We could constrain the solar system evolution based on this observation. However, there are still many unsettled issues concerning the ^{54}Cr anomalies, the accretion ages and the interpretation of the correlation. Here, we examine some of the most important issues.

^{26}Al Heterogeneity: Homogeneous distribution of ^{26}Al is assumed for calculating accretion ages of chondrites parent bodies. It is also assumed for estimating accretion ages of differentiated meteorite parent bodies. But, at present heterogeneous distribution of ^{26}Al [2] cannot be ruled out. Comparison of precisely determined Al-Mg ages and other ages is needed to solve this problem.

Exceptions: The NWA011 group (basaltic achondrites) and Tafassasset (primitive achondrite) do not fit the correlation. They both have high ^{54}Cr excesses [3,4] similar to that of CR chondrites and yet apparently formed early when there was enough ^{26}Al . A possible explanation may be that early-formed planetesimals in the terrestrial-planet formation region were gravitationally scattered into the far end of the asteroidal belt, capturing CR-like materials. This is an ad hoc explanation but is shown to be possible by numerical simulations [5].

CAIs: CAIs have ^{54}Cr , ^{50}Ti and ^{48}Ca isotope anomalies which are larger than those found in bulk meteorites. ^{54}Cr and ^{50}Ti anomalies in CAIs and bulk meteorites appear to be well correlated with each other [6] but ^{48}Ca anomalies are not so well correlated with them [7]. Since CAIs formed early, they do not fit the trend formed by various meteorites on the ^{54}Cr vs. accretion age diagram. If we consider that the isotope anomalies of neutron-rich isotopes in CAIs and bulk meteorites originated from a similar source, then, a kind of chemical fractionation that enriched carriers of the neutron-rich isotopes must have operated during CAI formation. Otherwise, the anomalies in CAIs may have originated from a totally different source.

Other issues such as the way to estimate accretion ages of differentiated meteorite parent bodies will also be discussed at the meeting.

References

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Keywords: ^{54}Cr , accretion age, meteorite parent bodies

Condensation and gas-solid experiments of minerals in protoplanetary disk conditions

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Condensation from vapor and gas-solid reaction may have been responsible for dust formation in the high-temperature region or during high-temperature events in the early solar system. Physical properties of condensed materials, such as size of individual components and textural relationship in a mineral assemblage, are important because they may change the efficiency of physical separation of dust and the interaction between dust and a radiation field, i.e., the thermal condition of the dust-forming environment. These properties are determined by reaction processes, but equilibrium calculations cannot deal with processes of reactions. It is thus crucial to understand condensation and gas-solid reaction processes of minerals and their kinetic aspects to understand the evolution of solar system materials. There have been many experimental studies on evaporation of major minerals in chondrites such as forsterite, enstatite, metallic iron, and troilite, while it has not been easy to carry out condensation and gas-solid experiments under low-pressure conditions for quantitative discussion on kinetic processes due to experimental difficulties. However, recent progresses of experimental studies have made it possible to determine the growth kinetics of minerals in chondrites. Here we report our recent condensation and gas-solid reaction experiments and the growth kinetics of minerals from vapor obtained in the experiments.

Keywords: dust, condensation, kinetics, protoplanetary disk

Chemical evolution of the atmosphere of Neptune and Jupiter induced by the cometary impact

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Gases produced after the collision of comet or asteroid in the atmosphere of giant planets, such as carbon monoxide, hydrogen cyanide, and sulfur compounds have key information to reveal the distribution and composition of minor bodies which exists in the outer solar system and the atmospheric evolution of gas giants. From the observational result, a collision of comet Shoemaker-Levy/9 on Jupiter in 1994 had produced large amount of short-lifetime volatile gases. Similar supplying process is predicted to be existed in the atmosphere of Neptune from the observational results that CO, which is not considered as a main reservoir of carbon, exists with high mixing ratio. In this presentation, I am presenting our observational results toward Neptune using ASTE telescope of NAOJ to constrain such supplying system and a new implication that the short-time variation of collision-induced gases in Jupiter using 45-m telescope.

Keywords: Radio astronomy, Jupiter, Neptune, Comet, Collision, Atmospheric evolution