

分子動力学シミュレーションにおける気相からの核生成過程：付着確率の効果 Nucleation process from vapor due to molecular dynamics simulations: effect of the sticking probability

田中 今日子^{1*}, 河野 明男², 田中 秀和¹

TANAKA, Kyoko^{1*}, KAWANO, Akio², TANAKA, Hidekazu¹

¹ 北海道大学低温科学研究所, ² 独立行政法人海洋研究開発機構 地球内部ダイナミクス領域

¹Institute of Low Temperature Science, Hokkaido University, ²Institute For Research on Earth Evolution, Japan Agency for Marine-Earth Science and Technology

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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Keywords: nucleation process, water, condensation, MD simulation

航空機による微小重力環境を利用した核生成の“その場”観察実験 In-situ observation of nucleation process under microgravity by an aircraft

木村 勇気^{1*}, 田中 今日子², 三浦 均¹, 塚本 勝男¹, 稲富裕光³

KIMURA, Yuki^{1*}, TANAKA, Kyoko², MIURA, Hitoshi¹, TSUKAMOTO, Katsuo¹, Yuko Inatomi³

¹ 東北大学, ² 北海道大学, ³ 宇宙航空研究開発機構

¹Tohoku University, ²Hokkaido University, ³JAXA

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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キーワード: 核生成, ダスト, ナノ粒子, その場観察

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ガス・ダスト系の熱的不安定 Thermal instability of gas-dust fluid system

渡辺 圭亮^{1*}, 中本 泰史¹
WATANABE, Keisuke^{1*}, NAKAMOTO, Taishi¹

¹ 東京工業大学地球惑星科学専攻

¹Department of Earth & Planetary Sciences, Tokyo Institute of Technology

ガス・ダスト二流体の系の一次元線形安定性解析を行った。本研究では放射冷却による熱的不安定に注目する。流体内のある領域でダストによる放射冷却が卓越すると、ガスの温度、圧力が低下し、この領域へ向けてガスの流れが発生する。この時、ガスの抵抗力によってダストもこの領域へ集められ、ダストの数密度が増加する。放射冷却率はダストの数密度に比例するため、より放射冷却が卓越する。この過程は一方向的であり、不安定である。

初期状態として、定常な、ガス温度がダスト温度より高い系を考える。定常状態を保つため、ガスの温度、密度の関数である仮想的なガスの熱源関数を導入し、冷却源としてダストからの放射冷却を考える。放射は吸収されることなく系の外へ放出されるとする。二流体の間でのエネルギーの輸送はガス・ダスト間の衝突によって起こり、運動量の輸送はガス・ダスト間の抵抗力によって起こると考える。

線型安定性解析の結果、分散関係式が得られた。またこれから、熱源関数のガス温度微分、およびガス密度微分がある条件を満たす時、不安定のモードが現れることがわかった。この時、ダストの密度の揺らぎは成長し、ダスト密度は増加する。

この結果は、原始惑星系円盤内で、現実的な熱源関数が不安定の条件を満たす場合に、ダスト集積が起こり得ることを示唆している。ダスト集積は微惑星形成に至るための重要な過程である。

キーワード: 線形安定性解析, ダスト集積, コンドリュール形成, 微惑星形成

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

54 クロムの異常と隕石母天体の集積年代 Cr-54 anomalies and accretion ages of meteorite parent bodies

杉浦 直治^{1*}, 藤谷 渉¹
SUGIURA, naoji^{1*}, FUJIYA Wataru¹

¹ 東京大学理学系研究科

¹Department of Earth and Planetary Sci. University of Tokyo, Tokyo, Japan

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.

26Al 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.

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キーワード: 54 クロム, 集積年代, 隕石母天体

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

原始惑星系円盤条件での鉱物の凝縮およびガス反応実験 Condensation and gas-solid experiments of minerals in protoplanetary disk conditions

橋 省吾^{1*}, 瀧川 晶¹, 永原 裕子¹, 小澤 一仁¹

TACHIBANA, Shogo^{1*}, TAKIGAWA, Aki¹, NAGAHARA, Hiroko¹, OZAWA, Kazuhito¹

¹ 東京大学大学院理学系研究科地球惑星科学専攻

¹Dept. Earth Planet. Sci., Univ. Tokyo

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.

キーワード: ダスト, 凝縮, 速度論, 原始惑星系円盤

Keywords: dust, condensation, kinetics, protoplanetary disk

小天体衝突がガス惑星大気進化に与える影響 - 電波望遠鏡を用いた観測的アプローチを中心として -

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

飯野 孝浩^{1*}, 水野 亮¹, 長浜 智生¹, 前澤 裕之¹, 森部 那由多¹, 桑原 利尚¹

IINO, Takahiro^{1*}, MIZUNO, Akira¹, NAGAHAMA, Tomoo¹, MAEZAWA, Hiroyuki¹, MORIBE, Nayuta¹, KUWAHARA, Toshihisa¹

¹ 名古屋大学 太陽地球環境研究所

¹ STEL, Nagoya University

小天体衝突はガス惑星の大気組成に大きな影響を与える。また、衝突時に生成される分子種やその全量、化学進化の過程を調べることは、その場観測が困難な小天体の分布やその組成の理解につながる重要なアプローチである。海王星大気中に高濃度で存在する一酸化炭素の存在は、その供給源として小天体衝突など外部からの輸送の存在を示唆している。我々は衝突時に生成される分子種のうち、硫化物に着目して研究を行なっている。彗星及び惑星中に含まれる硫化物が衝突時の高温高圧環境により分解された後、どの硫化物として観測されるかは、惑星大気及び彗星の組成を反映していることが強く示唆されている。ガス惑星中の硫化物の分子種やその寿命を調べることにより、多くの小天体を重力的に束縛しているガス惑星ならではの大气進化パスを明らかにすることが可能となる。我々はこれまで国立天文台野辺山のASTE電波望遠鏡及び45m電波望遠鏡を用い、ガス惑星大気に含まれる衝突時生成物質の観測を行ってきた。一連の観測から、生成物質の種類に制限を与えるとともに、その寿命が短期的に変動している可能性が示唆されつつある。本発表では、これまでの観測成果および衝突時生成物質の化学進化についての現状の成果について発表する。

キーワード: 電波天文学, 木星, 海王星, 彗星, 衝突, 大気進化

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