On the isotopic fractionation of terrestrial xenon by gravitational separation inside porous planetesimals with size distribution

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Taking account of the size distribution of planetesimals inferred from recent theoretical studies of planetesimal accretion, we examine gravitational separation of noble gases inside large porous planetesimals in the solar nebula. The size distribution is characterized by the value of the minimum planetesimal size \( R_0 \) for a given power-law distribution, which also determines the maximum planetesimal size for a given total mass of planetesimals. Both enrichment and isotopic fractionation of noble gases strongly depend on the value of \( R_0 \), as it determines the number of large planetesimals inside which gravitational separation of noble gases is significant. We find the ranges of the values of \( R_0 \) that can produce the enrichment and the isotopic fractionation of Xe similar to the terrestrial values separately, but the two ranges are found not to overlap. We also find significant isotopic fractionation of Kr for the parameter value that can produce the terrestrial isotopic fractionation of Xe, in contrast to the observation. These results suggest that the isotopic fractionation of terrestrial Xe cannot be explained if we only consider the gravitational separation inside porous planetesimals with the size distribution.

Keywords: atmosphere, composition, planetary formation, planetesimals, origin, solar system, terrestrial planets

INTRODUCTION

Elemental and isotopic abundances of noble gases have been measured for various materials, including the Earth’s atmosphere and various mantle-derived materials, meteorites, lunar samples, and the atmosphere of Mars and Venus. The similarities and differences among these observational data provide important constraints on the formation and evolution of the terrestrial planets and their atmospheres (e.g., Ozima and Podosek, 1983, 2002). However, there is still no satisfactory theory on the origin of terrestrial noble gases. In particular, there has been a long-standing interest in the elemental and isotopic composition of terrestrial Xe. The relative abundance of Xe in atmospheric noble gas is considerably lower than that in the noble gas component in meteorites. The relative deficiency of Xe in the Earth has been regarded to reflect some characteristic event during Earth’s evolution, and is called “the missing xenon paradox” (e.g., Pepin, 1991; Tolstikhin and O’Nions, 1994; Ozima and Podosek, 2002). On the other hand, observational data show that the Xe isotopic patterns of the Earth’s atmosphere and mantle-derived materials are practically identical, and heavier isotopes are enriched compared to the isotopic pattern of solar wind or meteorites. However, such distinct fractionation is not seen in the isotopic pattern of Kr (e.g., Ozima and Podosek, 2002). If we assume that the terrestrial atmosphere was derived from the primordial atmosphere with solar composition by some mechanism of mass fractionation such as hydrodynamic escape (e.g., Hunten et al., 1987), we would expect that Xe should be less depleted and less fractionated than lighter noble gases, such as Kr. Therefore, we have to explain why Xe is more depleted and isotopically fractionated, despite being heavier than Kr.

As a possible mechanism for creating the above noble gas patterns, Ozima and Nakazawa (1980) proposed fractionation caused by gravitational separation of solar nebula gases captured inside large porous planetesimals. In this model, the enhancement in the gas concentration increases exponentially with the atomic weight, thus isotopic fractionation becomes larger in heavier noble gas elements. When an isothermal nebula gas surrounds a constant porosity planetesimal of density \( \rho_s \) and radius \( R \), the enrichment factor \( \alpha_i \) of a noble gas species \( i \) with atomic mass \( \mu_i \) due to the gravitational separation can be written as (Ozima and Nakazawa, 1980)

\[
\alpha_i = 3 \exp(A\mu_i) \int_0^1 x^2 \exp(-A\mu_i x^2) dx,
\]
where $x = r/R$ is the distance from the center of the planetesimal scaled by $R$. The parameter $A$ is defined by

$$A = \frac{2\pi G m_i \rho_i R^3}{3kT},$$

where $m_i$ is the mass of a hydrogen atom, $k$ Boltzmann’s constant, and $T$ the temperature. Equation (1) shows that the enrichment becomes significant when $A\mu_i \approx 1$ (see Fig. 1). This condition can be rewritten as $R \approx R_{\text{crit}}$, where

$$R_{\text{crit}} = \left(\frac{3kT}{2\pi G m_{\text{H}} \rho_{\text{H}} \mu_i} \right)^{1/2}$$

is the critical radius derived by equating the pressure gradient of the gas species $i$ ($-kT\rho_{i}/(\mu_i m_{\text{H}} R^2)$) with the gravitational attraction by the planetesimal ($-\pi G \rho R^2 R$). For example, the values of $R_{\text{crit}}$ for Ne, Ar, Kr, and Xe are 580 km, 430 km, 280 km, and 230 km, respectively, where we assumed that $T = 225$ K and $\rho_{\text{H}} = 2$ g cm$^{-3}$ following Ozima and Nakazawa (1980). This is consistent with the results of Ozima and Nakazawa (1980; see their table 1), and they showed that the observed isotopic fractionation of terrestrial Xe could be explained by gravitational separation inside planetesimals of $R = 600$ km. However, in their model, Kr also showed non-negligible isotopic fractionation, in contrast to the observation.

In order to solve this problem, Igarashi and Ozima (1988) took account of a size distribution of planetesimals. On the basis of the results of the numerical simulation of planetesimal accumulation by Nakagawa et al. (1983), they assumed that the size distribution of planetesimals can be approximated by

$$N(R) = (R/R_0) \exp(-R/R_0) \quad (0 \leq R \leq R_{\text{max}}).$$

where $R_0$ is the radius at the maximum of $N(R)$. Fixing the values of $R_0$ to be in the range of 20–30 km ($R_0 = 30$ km in typical cases), Igarashi and Ozima (1988) calculated the isotopic fractionation of noble gases for several values of $R_{\text{max}}$. When $R_{\text{max}} = 10^3$ km, they were able to approximately reproduce the observed fractionation of terrestrial Xe, while leaving Kr and other lighter noble gases almost unfracticated. Igarashi and Ozima (1988) assumed the value of $R_0$ to be much smaller than $R_{\text{crit}}$ given by Eq. (3). As a result, the enrichment of Xe by the gravitational separation was caused mainly by a small number of large bodies near the high-mass end of the size distribution given by Eq. (4). On the other hand, they found that the total amount of heavy noble gases (i.e., Ar, Kr, and Xe) that could have been delivered to Earth in their model was too small (by two to three orders of magnitude) to account for terrestrial values. This was partly because the number of large bodies that can contribute to the noble gas enrichment (i.e., $R > R_{\text{crit}}$) was too small when the size distribution in the form of Eq. (4) with $R_0 = 20–30$ km is assumed. In fact, Takahashi (1999) studied the Xe enrichment by the gravitational separation for a wide range of values of $R_0$ and $R_{\text{max}}$ for the size distribution given by Eq. (4), and found that the enrichment factor can become comparable to or larger than the terrestrial values when $R_0 \approx 200$ km and $R_{\text{max}} \approx 850$ km. However, since both the enrichment and isotopic fractionation sensitively depend on the choice of $R_{\text{max}}$, she found that $R_{\text{max}}$ should be restricted in an unrealistically narrow range near $R_{\text{max}} \sim 850$ km to account for the terrestrial values.

As an alternative improvement of the model of Ozima and Nakazawa (1980), Zahnle et al. (1990a) took account of trapping of gravitationally fractionated gas at the critical pore-closing depth by lithostatic pressure. In this case, the isotopic fractionation is determined by the value of the critical pore-closing pressure that is a material property, thus Xe fractionation is roughly the same for all planetesimals large enough to close pores. On the basis of the data for sand and the lunar highland crust, Zahnle et al. (1990a) assumed that the critical pore-closing pressure to be 1–2 kbars, and found that the predicted degree of fractionation agrees with the terrestrial value. However, the total amount of Xe that could have been delivered to Earth in these planetesimals was more than an order of magnitude too small, unless rather efficient adsorption of Xe in small bodies and its release inside large planetesimals was assumed.

The size distribution (4) used by Igarashi and Ozima (1988) and Takahashi (1999) was based on the numerical simulation by Nakagawa et al. (1983). In this simulation, Nakagawa et al. found that a swarm of planetesimals ini-
tially of equal size would evolve such that the large bodies were always of nearly equal size (corresponding to $R_0$ in Eq. (4)) and that these large bodies contained most of the mass of the swarm. Such a mode of planetary growth is called “orderly growth.” On the other hand, later simulations by Wetherill and Stewart (1989, 1993) included the effect of equipartition of kinetic energy caused by gravitational scattering between planetesimals with different masses (which is called “dynamical friction”), which was neglected in Nakagawa et al.’s simulation. Wetherill and Stewart demonstrated that inclusion of this effect led to an alternative form of planetesimal growth termed “runaway growth,” in which a small number of large bodies grow much more rapidly than the remaining smaller bodies. The size distribution of the small bodies that contain most of the mass of the swarm in this stage can be approximately given by

$$n(m) dm \propto m^{-p} dm \quad (m_0 \leq m \leq m_{\text{max}}), \quad (5)$$

or, equivalently,

$$N(R) dR \propto R^{-q} dR \quad (R_0 \leq R \leq R_{\text{max}}), \quad (6)$$

where $m_0$ and $R_0$ are the initial values of the mass and radius of planetesimals before accretion, and $m_{\text{max}}$ and $R_{\text{max}}$ are those for the largest bodies in the planetesimal swarm. These results are also confirmed by N-body simulations (see a recent review by Kortenkamp et al., 2000). When fragmentation of planetesimals is taken into account, a number of bodies smaller than the initial size is produced. These small fragments have a shallower size distribution than the above size distribution of planetesimals formed by accretion (Eqs. (5) and (6)), and they could significantly contribute to the growth of runaway bodies in the late stage of accretion (Wetherill and Stewart, 1993; Ohtsuki et al., 2002). However, we neglect those small fragments in the present study, since the amount of noble gases captured inside planetesimals is significant only for large bodies.

In the present work, using the size distribution given by Eq. (5), which is inferred from recent theoretical studies of planetary accretion, we re-consider the problem of the Xe isotopic fractionation by gravitational separation inside porous planetesimals, by improving the model of Ozima and Nakazawa (1980) and Igarashi and Ozima (1988).

**GRAVITATIONAL SEPARATION INSIDE POROUS PLANETESIMALS WITH SIZE DISTRIBUTION**

**Method of calculation**

When the size distribution of planetesimals is expressed with $N(R) \ (R_0 \leq R \leq R_{\text{max}})$, the enrichment factor of a noble gas species $i$ in a protoplanet formed by accreting these planetesimals can be calculated as (Igarashi and Ozima, 1988)

$$\alpha_i = \frac{\int_{R_0}^{R_{\text{max}}} \alpha_i(R) N(R) R^2 \, dR}{\int_{R_0}^{R_{\text{max}}} N(R) R^2 \, dR}. \quad (7)$$

Isotopic fractionation is expressed in terms of $\delta$-values relative to the solar isotopic composition. In the case of Xe, $\delta$ is defined as

$$\delta_i = \left( \frac{^{130}\text{Xe}/^{130}\text{Xe}}{^{130}\text{Xe}/^{130}\text{Xe}} \right)_{\text{solar}} - 1. \quad (8)$$

Using $\overline{\alpha}_i$ defined by Eq. (7), $\delta_i$ can be written as (Igarashi and Ozima, 1988)

$$\delta_i = \frac{\overline{\alpha}_i}{\overline{\alpha}_{^{130}}} - 1. \quad (9)$$

When the size distribution of planetesimals is given

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by Eq. (5) or (6), the values of \( m_{\text{max}} \) can be approximately given by 
\( m_{\text{max}} \sim N_0^{3/5} m_0 \sim M_{\text{tot}}^{3/5} m_0^{3/5}, \)
where \( M_{\text{tot}} \) and \( N_0 \) are the total mass and the initial total number of planetesimals with mass \( m_0 \), respectively. This relation is consistent with the numerical results of Wetherill and Stewart (1989, 1993). Since \( M_{\text{tot}} \) is conserved in the course of planetesimal accumulation, the above relation provides a relation between \( m_0 \) and \( m_{\text{max}} \) given as 
\( m_{\text{max}}/m_0 \sim (M_{\text{tot}}/m_0)^{3/5}. \)
If we assume that \( M_{\text{tot}} = M_\odot \) and the material density of a planetesimal is given by \( \rho_s = 3 \text{ g cm}^{-3} \), we can rewrite this relation into the relation between \( R_0 \) and \( R_{\text{max}} \) given by
\[
R_{\text{max}}/R_0 = 200 \times \left( \frac{R_0}{1 \text{ km}} \right)^{-3/5}. \tag{10}
\]

In the above, we adopt 3 g cm\(^{-3}\) as the material density instead of 2 g cm\(^{-3}\) used in Ozima and Nakazawa (1980), as this value is often used in recent numerical simulation of planetary accretion (e.g., Wetherill and Stewart, 1993). The main results of the present work are not affected by the choice of this value.

The initial size of a planetesimal formed as a result of gravitational instability of the dust layer in the solar nebula is estimated to be several km, but significant uncertainty can be expected in the actual initial size of planetesimals. Therefore, we consider a rather wide range of values of \( R_0 \) (5–50 km), and corresponding values of \( R_{\text{max}} \) are calculated from the relation (10).

**Elemental fractionation**

Figure 3 shows the plots of \( \alpha_i \), defined by Eq. (7) as a function of \( R_0 \) (\( R_{\text{max}} \) is calculated by Eq. (10)) for four noble gas species. When \( R_0 \) is smaller than about 10 km, no significant enrichment is seen for all the four species.

The enrichment of Xe becomes significant when \( R_0 \approx 10 \) km. In this case, \( R_{\text{max}} \approx 500 \text{ km} \) (Eq. (10)), and a considerable number of planetesimals are larger than the critical size for Xe defined by Eq. (3). As a result, the enrichment of Xe becomes notable for \( R_0 \approx 10 \) km, while other lighter gases are less affected because their critical sizes are larger. We find that the enrichment of Xe becomes comparable to the observed value (~3 × 10\(^3\); Igarashi and Ozima, 1988; Ozima and Podosek, 1983) when \( R_0 = 30 \) km (\( R_{\text{max}} = 800 \) km), although \( \alpha_i \) depends quite sensitively on \( R_0 \) (Fig. 3). For this value of \( R_0 \), the enrichment factor of Kr is ~6, which is against the observation, while the enrichment of Ar and Ne is negligible.

**Isotopic fractionation**

Figure 4 shows the plots of Xe fractionation per a.m.u. as a function of \( R_0 \). We find rapid increase of the degree of fractionation with increasing \( R_0 \), although we note the change in the functional form, which reflects the different \( A\mu \)-dependence of \( \alpha \) (Fig. 1) for small and large bodies (i.e., \( A\mu \leq 1 \) and \( A\mu >> 1 \)). When approximated by a linear fractionation, the observed value of Xe fractionation per a.m.u. is \( \approx 0.04 \) (Ozima and Podosek, 1983). We find that the calculated value becomes comparable to the observed one when \( R_0 = 16–17 \) km, although again a quite sensitive dependence on \( R_0 \) is seen.

Isotopic fractionation lines calculated for various values of \( R_0 \) are shown in Fig. 5. As we have mentioned above, the isotopic fractionation pattern is similar to the observed fractionation of terrestrial Xe when \( R_0 = 16–17 \) km, except for \(^{129}\)Xe, whose excess can be attributed to the contribution of the decay of \(^{129}\)I (Ozima and Podosek, 1983). However, as the dependence of the slope on \( R_0 \) is so strong, changing the value of \( R_0 \) by several km results in completely different fractionation patterns (Fig. 5).
The results for the enrichment factor of Xe requires that \( R_0 \approx 30 \) km (Fig. 3), while those for its isotopic fractionation suggests \( R_0 = 16-17 \) km, and in both cases a slight change in the value of \( R_0 \) produces completely different results. Therefore, it seems difficult to produce the result that can explain both the elemental abundance and the isotopic fractionation of terrestrial Xe with the simple model considered in the above calculations.

In the above calculations, we assumed that a protoplanet (proto-Earth) accretes planetesimals with the size distribution given by Eq. (6). Exactly speaking, we have to multiply Eq. (6) with the collision rate between the protoplanet and a planetesimal with a given size, as the collision rate also depends on the size of a planetesimal through the weak size-dependence of the random velocity of planetesimals. If we assume that the random velocity is large enough to neglect the effect of the solar gravity during encounter and that the random velocity is determined by a balance between the gas drag from the solar nebula and gravitational scattering by the protoplanet (e.g., Wetherill and Stewart, 1993), we can show that the collision rate is proportional to \( m^{-1/5} \) or \( R^{-1/5} \), thus the value of \( q \) in Eq. (6) becomes 5.8, rather than 6. However, the mass-dependence of the random velocity and collision rate changes in different velocity regimes (e.g., Wetherill and Stewart, 1993; Ohtsuki et al., 2002). Taking these into account, we also calculated the enrichment and isotopic fractionation of Xe for various values of \( q \) in the range of \( 5.6 \leq q \leq 6.4 \) (Sano, 2000). Although a smaller value of \( q \) results in a relatively large number of large planetesimals (Eq. (6)) and thus facilitates the gravitational capture of noble gases, the results we found were similar to the above case with \( q = 6 \). The enrichment of Xe becomes comparable to the terrestrial value when \( 30 \text{ km} \leq R_0 \leq 35 \text{ km} \), and its isotopic fractionation becomes close to the observed value when \( 15 \text{ km} \leq R_0 \leq 20 \text{ km} \); again, the dependence on \( R_0 \) was quite sensitive.

**DISCUSSION**

In the present work, we investigated the fractionation of terrestrial Xe by gravitational separation inside porous planetesimals, taking account of the size distribution of planetesimals consistent with recent theoretical studies of planetary accretion. We find that the ranges of the parameter (i.e., the values of \( R_0 \)) that would account for the isotopic fractionation and the total amount of terrestrial Xe separately, but the dependence on \( R_0 \) was very strong and the two parameter ranges were found not to overlap. For the value of \( R_0 \) that results in the observed enrichment of Xe, significant enrichment of Kr was also found, in contrast to the observation. The derived values of \( R_0 \) (~15 km or ~30 km) were quite large compared to the initial size of planetesimals (~several km) inferred from the theory of the gravitational instability of the dust layer in the solar nebula (Goldreich and Ward, 1973). We assumed the gravitational equilibrium for the distribution of noble gases inside planetesimals (Ozima and Nakazawa, 1980; Igarashi and Ozima, 1988), but the time needed for diffusion to occur can be too long to verify this assumption, especially for smaller planetesimals (Zahnle et al., 1990a). Furthermore, the gravitational separation model has a difficulty that it alone cannot reproduce the observed abundance and isotopic composition of lighter noble gases in the terrestrial atmosphere. These results suggest that the fractionation of terrestrial Xe cannot be explained if we only consider the gravitational separation inside porous planetesimals with a size distribution, although it has been sometimes regarded as a promising mechanism (e.g., Ozima and Igarashi, 1989; Igarashi, 1995).

The other category of models for fractionating noble gas isotopes assumes vigorous hydrodynamic escape of a primordial atmosphere from Earth (e.g., Hunten et al., 1987; Sasaki and Nakazawa, 1988; Zahnle et al., 1990b; Pepin, 1991). Both gravitational separation and hydrodynamic models require the fractionated gases must be mixed with a source having low Xe/Kr ratio and unfractionated isotopic ratios (Dauphas, 2003). The mantle is assumed to be such a source in some models (e.g., Pepin, 1991), while others consider the contribution of an external component delivered by icy planetesimals, such as comets (e.g., Owen et al., 1992; Dauphas, 2003). The latter model depends on the experimentally observed depletion of Xe relative to Kr when trapped in amorphous water ice, and also on the assumption that the noble gas

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**Fig. 5. Isotopic fractionation lines of Xe for various values of \( R_0 \).** The isotopic fractionation pattern of Xe in the Earth’s atmosphere relative to the surface-correlated Xe in a lunar soil (which is regarded to be close to the solar Xe composition) is also shown by the dashed line, after Ozima and Podosek (1983).
isotopic composition of comets is solar. However, the dynamical history of comets and their noble gas composition are still unknown. The icy materials could have been delivered to the terrestrial planets in various ways, such as gas drag (e.g., Adachi et al., 1976) or radial diffusion due to gravitational scattering between planetesimals and protoplanets (e.g., Ohtsuki and Tanaka, 2003) during the early stage of the solar system evolution, and also as comets from the Uranus-Neptune region and the Kuiper Belt in the later stage (e.g., Morbidelli et al., 2000). Therefore, not only better understanding of the formation processes of the terrestrial planets, but also further understanding of the dynamical history and the composition of small icy bodies in the outer solar system will be necessary to clarify the origin and evolution of the atmospheres of terrestrial planets.

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