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Simulations of an isotopic fractionation by freezing in an open system

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Abstract This paper presents a model of isotopic fractionation by freezing under near-equilibrium conditions in an open system and uses the model to predict the fractionation curve and slope gradient of $\delta^{18}O$ versus δD. The simulation results show that 1) the fractionation curve and slope gradient are determined by the ratio of freezing rate to input rate, 2) the isotopic value in the initial stage of freezing is determined by the isotopic value of initial water; 3) in the latter half of freezing in an open system, the isotopic value converges to a certain value determined by that of input water. These results suggest that the shape of the fractionation curve is the method to distinguish whether freezing occurred in a closed or open system. This analysis is applied to an isotopic curve observed in basal ice of Hamna Glacier, Sôya drainage, East Antarctica. The isotopic curve indicates formation by regelation in an open system with a ratio of freezing/ input rates of about 10/ 4.

Key words simulation, isotopic fractionation, regelation, basal ice.

1 Introduction

Basal ice of glaciers and ice sheets has been widely studied to understand the inaccessible ice-bed interface (*e. g.*, Lawson 1979; Gow *et al*. 1979; Knight 1994; Hubbard and Sharp 1995, Souchez 1988). Use of stable isotopes of basal ice is a superior method to determine whether the basal ice was formed by melt-refreezing or non-melting at the inland base of glaciers and ice sheets. In a theoretical study of stable isotopes, Jouzel and Souchez (1982) showed that for a closed system, where no water is input or output, the slope gradient defined by $\delta^{18}O$ versus δD (hereafter, the freezing slope) depends on the initial composition of the liquid admitted to freeze (*e. g.*, equation 1 in Souchez and de Groote 1985). In contrast, the freezing slope in a open system depends on 1) the isotopic composition of the initial and input water and 2) the ratio of input to freezing rate (*e. g.*, equation 3 in Souchez and de Groote 1985). Freezing slopes of open and closed systems become similar when the isotopic composition of the input water is not significantly different from that of the initial water or when the freezing rate is much higher than the input rate. On the other hand, when the isotopic composition of the input water significantly differs from that of the initial water and when the ratio of input to freezing rate coefficient is high, the freezing slope is about 8 (Souchez and Jouzel 1984; Souchez and de Groote

1985). The freezing slope in the basal ice is a useful indicator to deduce whether water was input during freezing at the inland base of glaciers and ice sheets.

Iizuka *et al*. (2001) described the formation processes of the basal ice of Hamna Glacier, Sôya drainage, East Antarctica (hereafter the Hamna Basal Ice) from a detailed co-isotopic study. The basal ice consists of alternating layers of bubble-free and bubbly ice on the order of mm to cm in thickness. Isotopic curves were detected in the bubble-free ice layers and in some of the bubbly ice layers. According to the freezing slope, the ice layers having an isotopic curve were likely formed by regelation in an open system. To elucidate the circumstances of regelation in more detail for the area under Sôya drainage, I developed a model for an isotopic fractionation by freezing in the open system.

2 Model and simulation for isotopic fractionation by freezing

The model shown in Fig. 1 is one-dimensional and uses the fundamental equations in the method reported by Souchez *et al*. (1987). The model assumes that a water layer of thickness L freezes from one end to the other. Isotopic fractionation then occurs by freezing as follows: 1) the isotopic value of a newly-frozen piece of ice at point ΔL within the thickness L (= symbol $\delta^{18}O_{\Delta L(ice)}$ in Fig. 1) is determined both by the isotopic value of water before freezing at ΔL and by a coefficient for the isotopic fractionation; 2) the isotopic value of the water near point ΔL, which has a relatively lighter isotopic value due to the isotopic fractionation during freezing at ΔL (= symbol A in Fig. 1), is averaged immediately in the water that remains from ΔL to L (= symbol B in Fig. 1; assuming zero boundary layer thickness in the equations of Souchez *et al*. 1987); 3) the isotopic value in the ice is constant because the rate of diffusion in ice is much less than that in water.

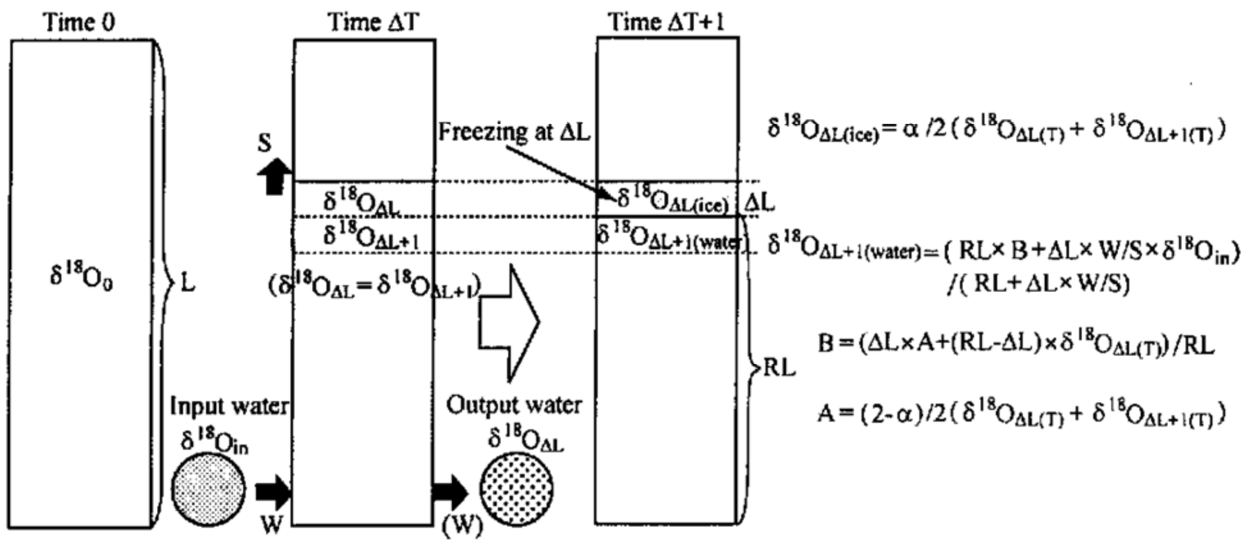

Fig. 1. A schematic diagram of the model. Left, center, right columns indicate the conditions before freezing (initial stage), before freezing at ΔL and after frozen at ΔL, respectively. White and gray boxes show water and frozen ice, respectively. The symbols and equations are explained in the text.

For the open system, input and output water are mixed with the remaining water during the freezing. The isotopic value of the remaining water is averaged immediately with that of the input water (= symbol$\delta^{18}O_{\Delta L(water)}$ in Fig. 1). I assume that the freezing and input rates are constant during freezing and that the output rate from the freezing system is equal to the input rate to the freezing system. This means that the volume of the remaining water in the freezing system is not affected by the existence of input and output water.

The simulation was done by using a difference equation method that divided the thickness L into 1000 layers (L = 1000 × ΔL). Input parameters for the simulation are 1) $\delta^{18}O_0$, the water's initial $\delta^{18}O$ value; 2) S, the water freezing rate; 3) $\delta^{18}O_{in}$, the input water's $\delta^{18}O$ value, and 4) W, the input rate of water. Both the $\delta^{18}O$ and the δD values were calculated, and then the freezing slopes were calculated using the fractionation curves of $\delta^{18}O$ and δD values. A negligibly slow rate of freezing (S: 0.1 mm/h) compared to the thickness (L: 30 mm) was used to satisfy the equilibrium condition in Lehmann and Siegenthaler (1991). The coefficients for isotopic fractionation were used 1.00291 for $^{18}O/^{16}O$ and 1.0210 for D/H (Lehmann and Siegenthaler 1991).

3 Simulation results and discussion of isotopic fractionation by freezing

Fig. 2 shows $\delta^{18}O$ as a function of freezing fraction for nine freezing/input rates (S/W). The curves show a clear distinction between closed and open systems. In a closed or nearly closed system (curves I and II), the fractionation curve decreases with freezing fraction slowly at first and then more rapidly, which agrees with Rayleigh-type fractionation. Conversely, in an open system with a high input rate (e.g., curve IX), the fractionation curve decreases very rapidly at first and then more slowly as the $\delta^{18}O$ (δD) value converges to fixed value in the last stage of freezing. Hence, the shape of the fractionation curve is determined by the S/W ratio and thus the freezing conditions; therefore, one can distinguish between closed and open systems by using the shape of the fractionation curve as the same manner as the freezing slope (Souchez and de Groote 1985).

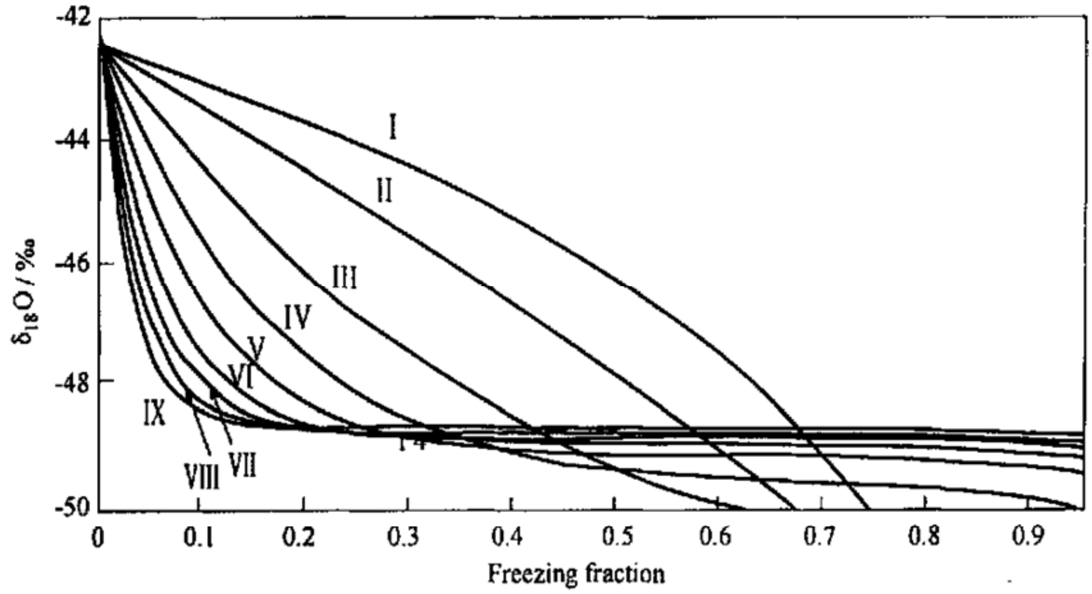

Fig. 2. Fractionation curves for several S/W ratios. The ordinate is $\delta^{18}O$ (‰) of the ice. The horizontal axis is the freezing fraction. I define the freezing fraction that ends before and after frozen are 0 and 1. Curves iv to ⑩ are for S/W equal to $10/x^2$ with x ranging from 0 to 8. The $\delta^{18}O_0$ and $\delta^{18}O_{in}$ are fixed at − 45 ‰ and − 48 ‰, respectively. The freezing slope are in Table 1.

Fig. 3 shows fractionation for various $\delta^{18}O_0$ values. $\delta^{18}O$ starts at the initial value and then can follow one of two different courses: the exponential decay that is characteristic of a closed system (curves ⅳ1 − ⅳ4), or a rapid approach to about − 45 ‰ for the open system. The latter value of about − 45 ‰ is determined by $\delta^{18}O_{in}$ value (discuss in next paragraph). If the $\delta^{18}O_0$ is changed, the $\delta^{18}O$ value in the initial stage of freezing is changed (curves 1 − 4). This result indicates that the $\delta^{18}O$ value in the initial stage of freezing is determined by the $\delta^{18}O_0$, although the $\delta^{18}O$ value depends also on the constant α, in strictly.

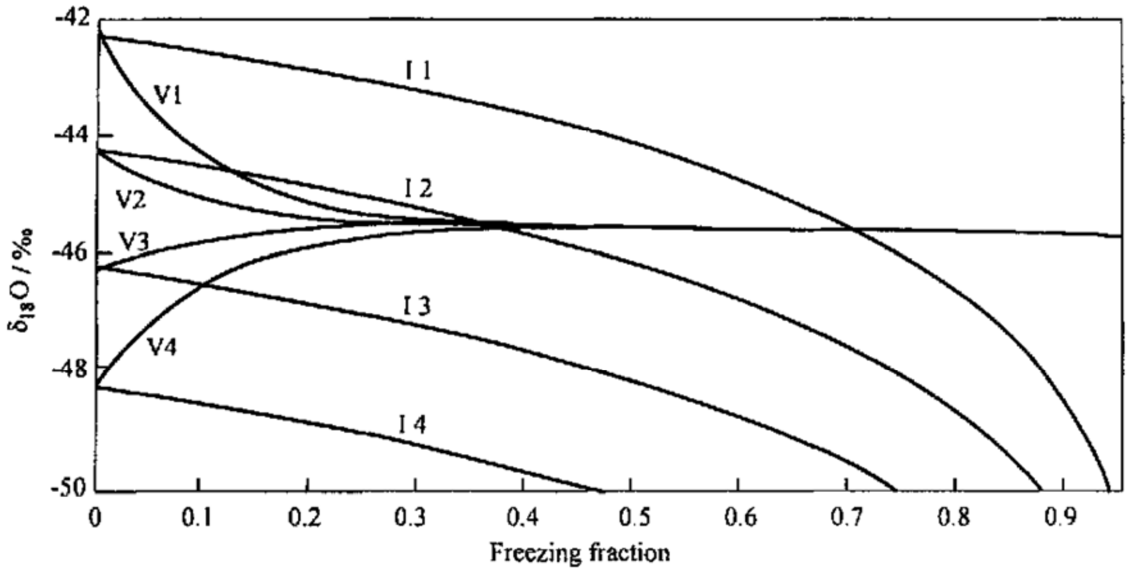

Fig. 3. Fractionation curves for four $\delta^{18}O_0$ values and closed and open systems. The ordinate is $\delta^{18}O$ (‰) of the ice and the abscissa is freezing fraction. $\delta^{18}O_0$ values are − 45 ‰ (top), − 47 ‰, − 49 ‰ and − 51 ‰ (bottom). Curves ⅳ1 − ⅳ4 have S/ W = 10/ 0 (closed system). Curves ㈨1 − ㈨4 have S/ W = 10/ 25 (open system). $\delta^{18}O_{in}$ is fixed at − 48 ‰. The freezing slope are in Table 2.

Fig. 4 shows that the fractionation depends on the $\delta^{18}O_{in}$ values. For example, after

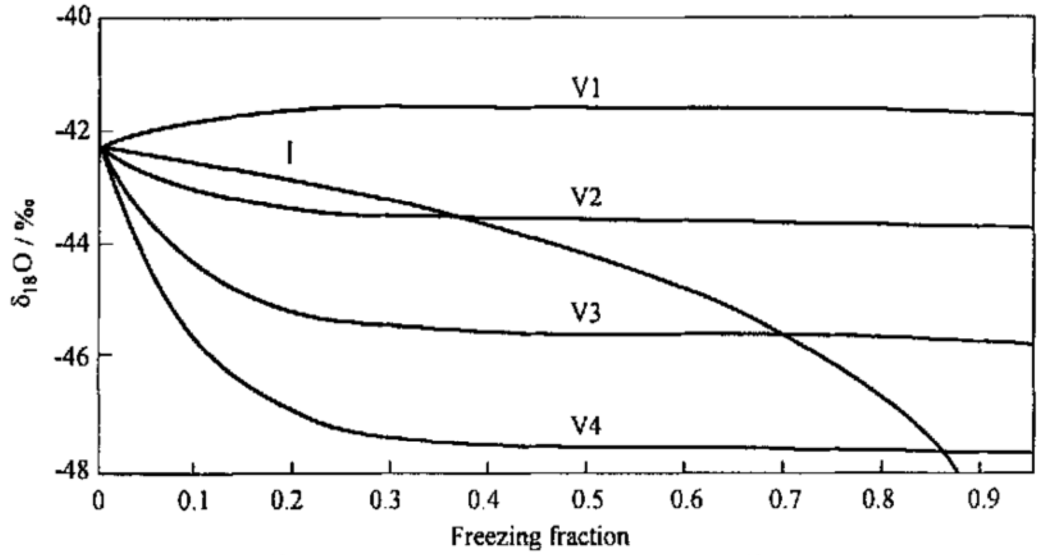

Fig. 4. Fractionation curves for $\delta^{18}O_0$ fixed at − 45 ‰. The ordinate is $\delta^{18}O$ (‰) of the ice and the abscissa is freezing fraction. Curves ㈨1 − ㈨4 all have S/ W = 10/ 25 and $\delta^{18}O_{in}$ of − 44 ‰ (top), − 46 ‰, − 48 ‰ and − 50 ‰ (bottom). Curves ⅳ has = 10/ 0. The freezing slope are in Table 3.

about 20% has frozen, the fractionation curves converge to values that increase with increasing $\delta^{18}O_{in}$ values (curves ㈨1 - ㈨4). The results indicate that these converged values are determined by $\delta^{18}O_{in}$.

Tables 1, 2 and 3 show the freezing slopes of the fractionation curves in Figs. 2, 3, and 4, respectively. The freezing slopes in Tables 1, 2, and 3 show the closed system (curve iv) have a slope of 5, whereas open system (curve ㈦ ㊂) have larger slopes that reach 8 for the most open systems. The two limits agree with previous theory: the value of 5 is the theoretical one found by Jouzel and Souchez (1982) for the closed system with $\delta^{18}O_0$ of about - 45 ‰ and δD_0 of about - 365 ‰, whereas, value of 8 is the theoretical value for an open system (Souchez and Jouzel 1984; Souchez and de Groote 1985). These simulations show that the shape of fractionation curve and the freezing slope are correlated. Thus, the shape of fractionation curve can be used to distinguish between closed and open systems without analyzing both $\delta^{18}O$ and δD.

Table 1. The S/W, $\delta^{18}O_0$, $\delta^{18}O_{in}$ and freezing slopes of the fractionation curves in Fig. 2

Curve No. in Fig. 2	iv	㈦	㈣	㈤	㈨	v		⑾	㊂
S/W	∞	10/1	10/4	10/9	10/16	10/25	10/36	10/49	10/64
$\delta^{18}O_0$/ ‰	- 45	- 45	- 45	- 45	- 45	- 45	- 45	- 45	- 45
$\delta^{18}O_{in}$/ ‰	- 48	- 48	- 48	- 48	- 48	- 48	- 48	- 48	- 48
freezing slope	5.0	6.3	7.2	7.6	7.8	7.8	7.9	8.0	8.0

Table 2. The S/W, $\delta^{18}O_0$, $\delta^{18}O_{in}$ and freezing slopes of the fractionation curves in Fig. 3

Curve No. in Fig. 3	iv1	iv2	iv3	iv4	㈨1	㈨2	㈨3	㈨4
S/W	∞	∞	∞	∞	10/25	10/25	10/25	10/25
$\delta^{18}O_0$/ ‰	- 45	- 47	- 49	- 51	- 45	- 47	- 49	- 51
$\delta^{18}O_{in}$/ ‰					- 48	- 48	- 48	- 48
freezing slope	5.0	4.9	4.8	4.6	7.9	7.5	7.9	7.9

Table 3. The S/W, $\delta^{18}O_0$, $\delta^{18}O_{in}$ and freezing slopes of the fractionation curves in Fig. 4

Curve No. in Fig. 4	iv	㈨1	㈨2	㈨3	㈨4
S/W	∞	10/25	10/25	10/25	10/25
$\delta^{18}O_0$/ ‰	- 45	- 45	- 45	- 45	- 45
$\delta^{18}O_{in}$/ ‰		- 44	- 46	- 48	- 50
freezing slope	5.0	7.9	7.5	7.8	7.9

Table 4. The S/W, $\delta^{18}O0$, $\delta^{18}Oin$ and freezing slopes of the fractionation curves in Fig. 6. Roman numerals are for calculated curves, circled numbers are for data curves

Curve No. in Fig. 4	iv	㈦	㈣	㈤			④	㈣	
S/W	∞	10/1	10/4	10/9	10/36	(∞)	(10/1)	(10/4)	(10/9)
$\delta^{18}O_0$/ ‰	- 45.0	- 45.0	- 45.0	- 45.0	- 45.0	(- 45.0)	(- 45.0)	(- 45.0)	(- 45.0)
$\delta^{18}O_{in}$/ ‰	- 48.4	- 48.4	- 48.4	- 48.4	- 48.4	(- 48.4)	(- 48.4)	(- 48.4)	(- 48.4)
freezing slope	5.0	6.4	7.3	7.5	8.0	7.7	7.7	7.7	7.7

4 Comparison of the simulation results with isotopic curve observed in the Hamna basal ice

To apply the above analysis, I compare the simulation results with a typical isotopic curve from the Hamna basal ice. Fig. 5 shows the $\delta^{18}O$ profile at about 1.7 m above the bedrock in the Hamna basal ice. The isotopic curve at the thickness 723 mm in Fig. 5 was suggested to formed by a single melt-refreezing (Iizuka *et al*., 2001). The reason why this isotopic curve is selected as a typical example, is that the curve has one of the most isotopic samples (15 samples) within a single decreasing observed in the Fig. 6 of Iizuka *et al*. (2001). The maxima $\delta^{18}O$ value is − 42.3 ‰ at 7 mm, and the minima is − 45.7 ‰ at 23 mm. Assuming that the $\delta^{18}O$ values in the initial and last stages of the freezing are determined by the $\delta^{18}O_0$ and $\delta^{18}O_{in}$ values (Figs. 3 and 4), the $\delta^{18}O_0$ and $\delta^{18}O_{in}$ values are − 45.0 ‰ and − 48.4 ‰, respectively.

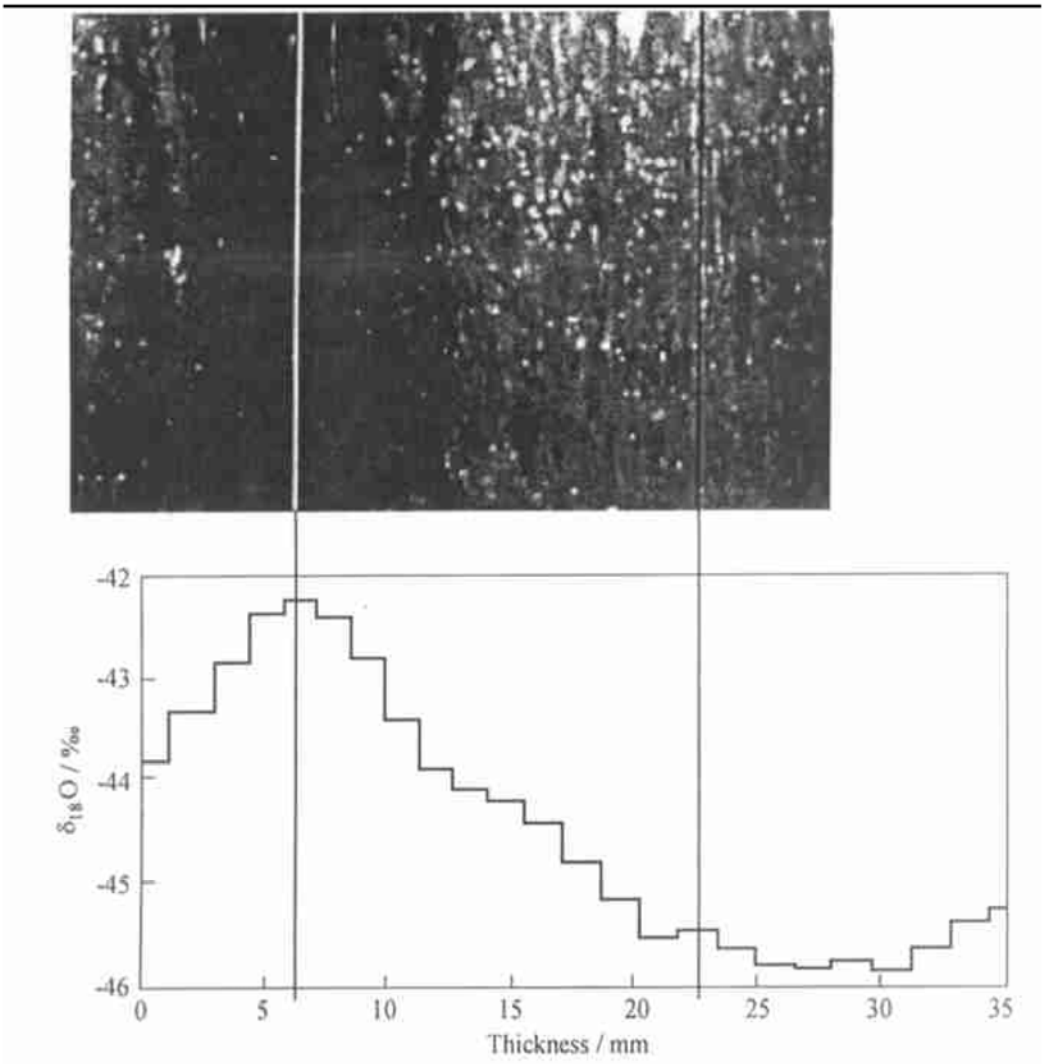

Fig. 5. Photograph taken by reflected light and $\delta^{18}O$ profile at about 1.7 m above the bedrock in the Hamna basal ice. The thickness 7– 23 mm in Fig. 5 equals to the thickness 122– 138 mm in Fig. 8 of Iizuka *et al*. (2001), and is used as a measured fractionation curve. Black and white parts in the photograph indicate the bubble-free and bubbly layers, respectively.

Fig. 6 shows isotopic curves for the Hamna basal ice ((1) − (4)) and simulation results for various S/W values when the $\delta^{18}O_0$ and $\delta^{18}O_{in}$ values are − 45.0 ‰ and − 48.5 ‰, respectively (iv– ㊄and). Because the relation between position in the ice and freezing fraction is not known, four cases are shown. In the first case ( ), the point at 23 mm is assumed to have a freezing fraction of 1.0. For cases (2) − (4), the corresponding freezing fractions at 23 mm are 0.65, 0.45, and 0.35. Curve (1) decreases logarithmically with freezing, which indicates an open system, whereas curve iv decreases exponentially. Curve (2) decreases faster than that of curve ㊆ whereas, curve (4) decreases more slowly than that of curve ㊄ Hence, the data in curves (1), (2), and (4) are not fit to theory.

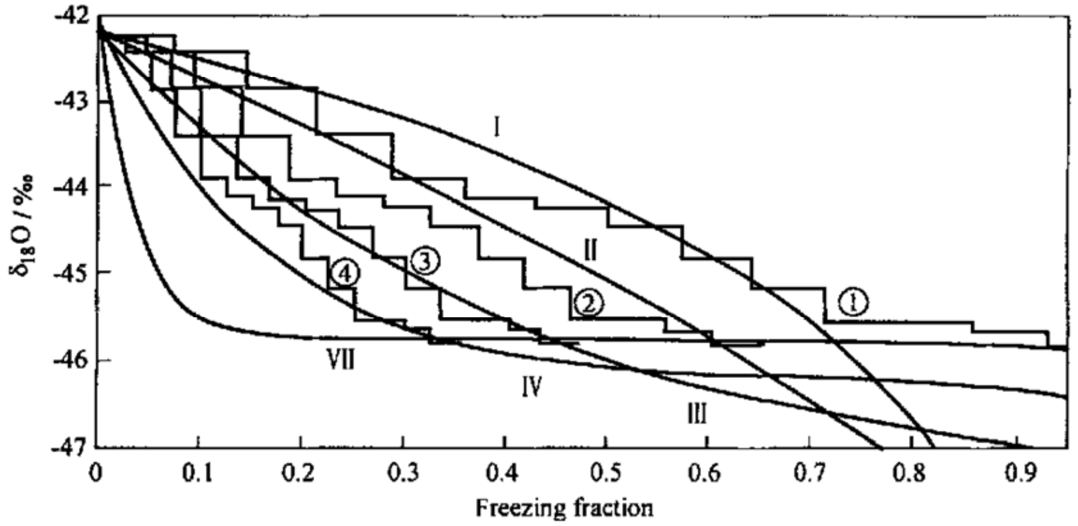

Fig. 6. Calculated fractionation curves (thin line) and measured fractionation curves from the Hamna Basal ice (thick lines). The ordinate is $\delta^{18}O$ (‰) of the ice and the abscissa is freezing fraction. A single measured curve is plotted for four final freezing fractions, curves – . Calculated curves iv– ㊄and have S/W = $10/x^2$ with x = 0 – 3 and 6, respectively. $\delta^{18}O_0$ and $\delta^{18}O_{in}$ are fixed at – 45.0 and – 48.4 ‰, respectively. The freezing slope are in Table 4.

The isotopic curve (3) fits the theoretical curve ㊃ which has S/W = 10/4. This result suggests that regelation was performed in the open system with the circumstance of 10/4 for the S/W. Furthermore, the calculated freezing slope with this value of S/W is about 7.9 (Table 4), which agrees with the value of 7.8 for the isotopic curve in the Hamna basal ice.

5 Concluding remarks

I developed a model for isotopic fractionation by freezing in an open system under the assumptions of near equilibrium condition and zero boundary-layer-thickness. The simulation results showed that 1) the shape of the fractionation curves and the slope of $\delta^{18}O$ vs. δD are determined by the ratio of freezing/input rates, 2) the isotopic value in the initial stage of freezing is determined by isotopic value of initial water, and 3) if the freezing system is open, the converged isotopic value in the last stage of the freezing is determined by the isotopic value of the input water. The simulation results suggest that an ice-water system that freezes as an open system can be distinguished from that of the closed system two ways: using the slope of $\delta^{18}O$ and δD, as proposed by Souchez and de Groote (1985), and also by the shape of the fractionation curve. The shape of fractionation curve can be used to distinguish between closed and open systems without analyzing both $\delta^{18}O$ and δD.

This model was used to analyze a measured isotopic curve from the Hamna basal ice. The shape of the isotopic curve fit the theoretical curve when S/W equaled 10/4, which indicates that this ice formed as an open system with a ratio of the rate of freezing to the input water of 10/4. The model will be used in further studies to interpret freezing conditions in basal ice through measured fractionation curves and thus help to determine refreezing conditions at the bases of ice sheets and glaciers.

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