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THEORETICAL ANALYSIS OF OXYGEN DIFFUSION AT STARTUP IN AN ALKALI METAL HEAT PIPE WITH GETTERED ALLOY WALLS

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16. Abstract

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THEORETICAL ANALYSIS OF OXYGEN DIFFUSION AT STARTUP IN AN ALKALI METAL HEAT PIPE WITH GETTERED ALLOY WALLS

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SUMMARY

The diffusion of oxygen into, or out of, a gettered alloy exposed to oxygenated alkali liquid metal coolant, a situation arising in some high temperature heat transfer systems, was analyzed. The relation between the diffusion process and the thermochemistry of oxygen in the alloy and in the alkali metal was developed by making several simplifying assumptions. The treatment is therefore theoretical in nature. However, a practical example pertaining to the startup of a heat pipe with walls of T-111, a tantalum alloy, and lithium working fluid illustrates the use of the figures contained in the analysis.

INTRODUCTION

Refractory metal alloys have been proposed for use at high temperatures in structures for space power production and other applications. When alkali metal coolants are present, oxygen in the system components must be minimized or segregated if corrosion is to be avoided. One means of segregating oxygen in refractory metal alloys has been the use of a gettering metal. To getter oxygen, hafnium has been introduced into tantalum-8 tungsten (wt. %) alloys to form T-111 (tantalum-8 tungsten-2 hafnium). Because of the stability of hafnium dioxide (HfO_2), most of the oxygen present in, or entering, the alloy will be sequestered as HfO_2 until all the hafnium is consumed.

In some applications involving gettered alloys, the oxygen levels to which the alloy is exposed may vary sharply. For instance, in a new heat pipe with alkali metal working fluid, the refractory metal wicking, arteries and walls contain oxygen introduced in all the fabrication processes. At startup, the liquid metal purified by distillation from the evaporator condenses on the condenser walls and is entrained in the wicking and arteries. The chemical potential of oxygen in these parts is very likely to be higher than that of the oxygen in the liquid metal, and oxygen will be leached into the liquid and transported to the evaporator. Because the liquid metal vapor can contain little oxygen, the concentration in the liquid metal of the evaporator may rise. As this concentration rises, the oxygen can move into the evaporator walls. If the concentration of oxygen in the evaporator wall becomes sufficiently high over a period of time, corrosive failure of the wall is a probability (ref. 1).

Refractory alloys containing tantalum and niobium can dissolve considerable amounts of oxygen (ref. 2) and diffusion at elevated temperatures is rapid (ref. 3). The presence of a gettering element as an oxygen sink in alloys of tantalum and niobium can be expected to modify both the rate of diffusion with time, and the oxygen capacity of the alloy.

In this report a simple analysis of the oxygen diffusion process into, or out of, a gettered alloy exposed to oxygenated liquid alkali metal is presented. The analysis relates the thermochemistry of oxygen in the liquid metal and in the container metal, to the diffusion into or out of a semi-infinite alloy. The analysis is intended to clarify some of the features of the diffusion processes process which may be encountered in cooling systems using gettered refractory alloys and alkali liquid metals. For this purpose, an example is presented for oxygenated lithium in contact with T-111, a gettered tantalum alloy chosen because it is being considered for use in heat pipes. The analysis is part of a continuing study of gettering systems for use in heat pipes.

ANALYSIS

Figure 1, from reference 4, shows a computed distribution of oxygen between lithium and tantalum under conditions of equilibrium. At any given point on figure 1, oxygen in the tantalum at atom fraction $x_{O(Ta)}$ has the same chemical potential as oxygen in the dilithium oxide (Li_2O) at mole fraction x in lithium. Experimental determinations of the solubility of oxygen in lithium and in tantalum, extended analytically, were used in thermochemical calculations to construct figure 1. Figure 1 must therefore be regarded as largely theoretical. While the distribution shown has not been substantiated by experimental data, it will be used here for purposes of illustration.

The atomic fraction of oxygen in tantalum against the mole fraction of Li_2O in solution with lithium is shown for several temperatures. Also shown in figure 1 is a crossed-hatched area representing the zone of stability for HfO_2 computed as though metallic hafnium were in a phase separate from tantalum. The data for HfO_2 were replotted from reference 5. Actually, the hafnium in dilute solution in an alloy such as T-111 will have a chemical potential somewhat different from the pure hafnium metal (ref. 6). The effect of this change in the chemical potential of hafnium on the location of the hatched area is no doubt of less consequence than some of the other assumptions entering into the construction of figure 1 (ref. 4).

In the simple model of a diffusion event considered here, the alloy is assumed to be of semi-infinite extent in the u direction (fig. 2(a)). This assumption is made in order to simplify the mathematics. The initial concentration of oxygen throughout the alloy is c_∞, taken here in units of density, or grams per cubic centimeter. At time $t = 0$ conditions external to the alloy are suddenly changed, such that the concentration of oxygen required for equilibrium in the alloy is c_0. Exposure to oxygen-bearing lithium could bring about such a change in conditions. If c_0 exceeds the oxygen concentration c_g at which the gettering metal oxide is stable, the oxide is formed by the diffusion of oxygen at a rate governed by the diffusion constant D.

The assumption is made that c_0 is below the concentration required for oxidation of the main alloying constituents (tungsten and tantalum in T-111). Any formation and precipitation of the oxide of the gettering metal is assumed to have negligible effect on the diffusion coefficient D. When the concentration c_g is reached at any point in the alloy, the getter is assumed to be oxidized at a sufficiently rapid rate that chemical equilibrium is maintained locally.

The method of attacking the present problem was adapted from techniques used by Crank (ref. 7) for mass diffusion in which the diffusion constant is discontinuous with concentration. This method is similar to that used by Danckwerts (ref. 8) for the general case of heat transfer with a moving boundary, as in the freezing of ice.

The time-dependent differential equation for diffusion in one dimension is

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial u^2} \tag{1}$$

Referring to figure 2, one solution pertains to the region $c_g < c < c_0$, designated by subscript 1;

$$c_1 = c_0 + A \operatorname{erf} \frac{u}{2\sqrt{Dt}} \tag{2}$$

The other pertains to the region $c_\infty < c < c_g$, designated by subscript 2;

$$c_2 = c_\infty + B \operatorname{erfc} \frac{u}{2\sqrt{Dt}} \tag{3}$$

where c is the oxygen concentration, u is the distance coordinate, t is time, erf z designates the error function, and erfc z = 1 - erf z is the complementary error function.

Figure 2(a) presents a schematic view of conditions during the precipitation of gettering metal oxide. A lamina of thickness Δu is shown at the concentration c_g, within which precipitation of getter oxide is occurring. The flux of oxygen into the lamina is $-D(\partial c_1/\partial u)$ and the flux out is $-D(\partial c_2/\partial u)$, both in grams per square centimeter per second or comparable units. If the reaction between getter X and oxygen is

$$mX + nO \rightarrow X_mO_n \tag{4}$$

and the concentration of getter in the alloy is c_m (g/cm^3), the oxygen gettering capacity of the alloy is

$$q = -c_m \frac{n}{m}\frac{M_O}{M_X} \ (\mathrm{g/cm^3}) \tag{5}$$

exclusive of the oxygen dissolved in the major alloy constituents. The negative sign indicates the consumption of free oxygen, and M denotes molecular weight.

If $q\ \Delta u$ grams of free oxygen are consumed in the lamina, the oxygen consumed must be represented by the net diffusional influx into the lamina during the time span Δt, or

$$\left(D\frac{\partial c_1}{\partial u} - D\frac{\partial c_2}{\partial u}\right)_{c_g} \Delta t = q\ \Delta u \tag{6}$$

The lamina must move with velocity $V_g = \Delta u/\Delta t$ to encounter fresh getter material. Thus equation (6) in the limit gives a condition for the boundary between regions 1 and 2:

$$D\left(\frac{\partial c_1}{\partial u}\right)_{c_g} - D\left(\frac{\partial c_2}{\partial u}\right)_{c_g} = q\ V_g \tag{7}$$

At the gettering concentration c_g occurring at $u = u_g$, both c_1 in equation (2) and c_2 in equation (3) must equal c_g. Therefore equation (2) becomes

$$c_g = c_o + A\ \mathrm{erf}\ \frac{u_g}{2\sqrt{Dt}} \tag{8}$$

and equation (3) becomes

$$c_g = c_\infty + B \operatorname{erfc} \frac{u_g}{2\sqrt{Dt}} \tag{9}$$

Since c_g is constant, the variable $u_g/2\sqrt{Dt}$ must be constant. Defining

$$\kappa = \frac{u_g}{2\sqrt{Dt}} \tag{10}$$

enables equations (8) and (9) to be solved for A and B as follows:

$$A = \frac{c_g - c_o}{\operatorname{erf} \kappa} \tag{11}$$

$$B = \frac{c_g - c_\infty}{\operatorname{erfc} \kappa} \tag{12}$$

Equations (2), (3), (11), and (12) with a little manipulation can be expressed as

$$\frac{c_1 - c_\infty}{c_o - c_\infty} = 1 - \alpha \frac{\operatorname{erf} \frac{u}{2\sqrt{Dt}}}{\operatorname{erf} \kappa} \tag{13}$$

$$\frac{c_2 - c_\infty}{c_o - c_\infty} = \beta \frac{\operatorname{erfc} \frac{u}{2\sqrt{Dt}}}{\operatorname{erfc} \kappa} \tag{14}$$

where

$$\alpha = \frac{c_o - c_g}{c_o - c_\infty} \tag{15}$$

and

$$\beta = \frac{c_o - c_\infty}{c_o - c_\infty} = 1 - \alpha \tag{16}$$

Equation (13) applies only when $c_1 > c_g$, and equation (14) only when $c_2 < c_g$. The gettering front velocity from equation (10) is

$$v_g = \left(\frac{du_g}{dt}\right) = \kappa\sqrt{\frac{D}{t}} = \frac{2\kappa^2 D}{u_g} \tag{17}$$

Combination of equations (7), (10), (13), (14) and (17) results in an implicit expression for κ

$$\frac{1 - \beta}{\text{erf } \kappa} - \frac{\beta}{\text{erfc } \kappa} + \gamma \sqrt{\pi}\, \kappa e^{\kappa^2} = 0 \tag{18}$$

where

$$\gamma = \frac{-q}{c_0 - c_\infty} \tag{19}$$

Essentially, γ represents the relative gettering power of the alloy since it is the ratio of the oxygen gettering capacity to the uptake of uncombined oxygen required to achieve chemical equilibrium. Equation (17) can be solved iteratively for κ, with values of β and γ assigned.

Figure 3(a) shows κ for several values of β against γ from 10^{-1} to 10^2, while figure 3(b) shows κ against γ from 10^2 to 10^5. As the relative gettering strength γ increases, κ decreases, representing a slowing of the gettering front (eq. (17)).

With κ determined as a function of β and γ, equations (13) and (14) can be evaluated. Letting

$$z = \frac{u}{2}\sqrt{Dt} \tag{20}$$

equations (13) and (14) give

$$\frac{c - c_\infty}{c_0 - c_\infty} = 1 - \frac{\alpha \text{ erf } z}{\text{erf } \kappa} \qquad 0 < z \leq \kappa \tag{21}$$

$$\frac{c - c_\infty}{c_0 - c_\infty} = \beta \frac{\text{erfc } z}{\text{erf } \kappa} \qquad \kappa < z \leq \infty \tag{22}$$

Figure 4 shows the concentration function $(c - c_\infty)/(c_0 - c_\infty)$ plotted against z for β of 0, 0.2, 0.4, 0.6, and 0.8 and values of γ ranging from 10^{-1} to 10^5.

As γ; representing the gettering strength, increases, the break in the curves of $(c - c_\infty)/(c_0 - c_\infty)$ becomes more pronounced, as required by equation (7). When $\beta = 0$ as in figure 4(a), no material passes through the gettering front. For this reason the case $\beta = 0$ applies to one-dimensional diffusion in bodies of thickness y until the gettering front reaches y.

The total amount of oxygen contained in the structure at any time, per unit area, is given by

$$G = \int_0^{u_g} c_1\, du + \int_{u_g}^{\infty} c_2\, du - q\, u_g \tag{23}$$

where, c_1 is given by equation (13) and c_2 by equation (14). Integration of equation (23) and combination with equations (10), (18), and (19) gives

$$\frac{G}{2\sqrt{Dt}\,(c_0 - c_\infty)} = \frac{\alpha}{\sqrt{\pi}\,\operatorname{erf}\kappa} + 2\gamma\kappa \tag{24}$$

A plot of the dimensionless gettering parameter $G/2\sqrt{Dt}\,(c_0 - c_\infty)$ against γ for several values of β is shown in figure 5.

The foregoing development treated the diffusion of oxygen into an alloy. The same analysis and figures can also be applied to the outgassing of oxygen from a material containing uniformly distributed oxygen in excess of that required to oxidize the getter. In such a case $c_\infty > c_g > c_0$, and q (eq. (5)) is positive since the getter acts as a source rather than a sink. Figure 2(b) illustrates the situation. Figures 3, 4, and 5 are again applicable, with $G/2\sqrt{Dt}\,(c_0 - c_\infty)$ in figure 5 pertaining to loss of oxygen from the body.

EXAMPLE

The following example illustrates an application of the figures that have been presented. The example is based on the situation that might occur in the evaporator of a new heat-pipe. The refractory metal wick structure and arteries of alkali metal heat pipes often contain large amounts of oxygen after fabrication. At the first startup of the pipe, a large amount of oxygen from these sources and from the condenser walls is swept into the evaporator causing a sudden, large increase in the oxygen concentration of the alkali metal in the evaporator section of the pipe.

Consider an alloy with a composition within the range designated as T-111 (ref. 9). By weight, this alloy contains approximately 89.5 percent tantalum, 8 percent tungsten, 2.5 percent hafnium, 0.003 percent oxygen, 0.003 percent nitrogen, and 0.001 percent carbon. A semi-infinite section of this alloy is assumed to be heated to 1700 K and simultaneously exposed to solution of lithium and lithium oxide, with the mole fraction x of Li_2O in solution equal to 0.02. The problem will be to find β and γ and from these determine the time for the gettering front to move 1 millimeter and the time for $(c - c_\infty)/(c_0 - c_\infty)$ to reach 0.5. The amount of oxygen per square centimeter of structure when the front has penetrated 1 millimeter is to be found. The equilibrium distribution of oxygen between liquid lithium and tantalum in the alloy is to be taken from figure 1.

The assumption is made that any oxygen in the system must either be dissolved in the tantalum, or combined as HfO_2 and dissolved in the tantalum. The oxygen concentrations must be below the point at which tungsten oxides or Ta_2O_5 forms. The possible formation of lower oxides of hafnium is disregarded. The possible presence of negligible amounts of nitrides is also ignored.

The criteria for the distribution of oxygen in the alloy as fabricated are the following:

(1) When $C_O < c_g$, no HfO_2 is present and $c_\infty = C_O$. Here C denotes the total concentration of an element in the alloy, both combined and uncombined, after fabrication.

(2) When $c_g < C_O < 2C_{Hf}(M_O/M_{Hf})$, some amount of hafnium is oxidized and $c_\infty = c_g$. Moreover the effective gettering capability is reduced because some of the hafnium is already oxidized during fabrication. The amount of fabrication oxygen which must be taken up by hafnium is $C_O - c_g$. This reduces the gettering capability of the hafnium, and equation (5), modified to account for the fabrication oxygen, becomes

$$-q = 2C_{Hf}\frac{M_O}{M_{Hf}} - (C_O - c_g) \tag{25}$$

(3) When $C_O > 2C_{Hf}(M_O/M_{Hf})$, all hafnium is oxidized and no further gettering occurs.

The density ρ of T-111 is nominally 16.70 grams per cubic centimeter (0.604 lb/cu in.) (ref. 9). The total concentration of hafnium for the assumed composition, both oxidized and unoxidized, is

$$C_{Hf} = w_{Hf}\rho = 0.418 \text{ g/cu cm} \tag{26}$$

where w is the weight fraction of constituent in the alloy. The total concentration of oxygen is

$$C_O = w_O\rho = 5.02\times10^{-4} \text{ g/cu cm} \tag{27}$$

From figure 1, for 1700 K and a Li_2O mole fraction x of 0.02, $x_g = 3.1\times10^{-6}$ for monatomic oxygen dissolved in tantalum. Converting this to an oxygen concentration in the alloy gives

$$c_g = C_{Ta}\frac{M_O}{M_{Ta}}x_g = 4.1\times10^{-6} \text{ g/cu cm}$$

Also $2C_{Hf}\,(M_O/M_{Hf}) = 0.075$ gram per cubic centimeter from equation (26). Criterion 2 is thus satisfied, and $c_\infty = c_g = 4.1\times10^{-6}$ gram per cubic centimeter. From equation (25), $-q = 0.074$ gram per cubic centimeter.

The oxygen concentration c_0 represents equilibrium between the oxygen in the tantalum and in the lithium after the hafnium has all been consumed. From figure 1 for $x = 0.02$ and $T = 1700$ K, $x_{O(Ta)} = 6\times10^{-6}$. Then

$$c_0 = c_{Ta}\frac{M_O}{M_{Ta}}x_{O(Ta)} = 7.9\times10^{-6} \text{ g/cu cm}$$

Therefore, $c_0 - c_\infty = 3.8\times10^{-6}$ gram per cubic centimeter. From equation (16) $\beta = 0$ and from equation (19) $\gamma = 1.95\times10^4$. For these values of β and γ figure 3(b) gives a κ of 5×10^{-3}.

In order to compute the time for penetration of the gettering front to a selected depth from the foregoing value of γ, the diffusion coefficient for oxygen in T-111 must be specified. Reference 3 presents this equation for the coefficient of diffusion of oxygen in tantalum

$$D = 0.0044 \exp\left(-\frac{12\,800}{T}\right) \text{cm}^2/\text{sec} \tag{28}$$

At 1700 K, $D = 8.474\times10^{-3}$ square centimeter per hour. This value is accepted here for the T-111 alloy. Since $\kappa = 5\times10^{-3}$, the time for the gettering front to reach 1 millimeter (eq. (10)) is 1.2×10^4 hours.

From figure 4(a) a ratio $(c - c_\infty)/(c_0 - c_\infty)$ of 0.5 is reached at $z = 2.5\times10^{-3}$. For the diffusion coefficient just determined, the ratio of 0.5 is reached at 1 millimeter of depth after 4.7×10^4 hours, by equation (20). This value at first glance seems to represent an inordinately slow diffusion process in view of the 1700 K temperature. Three factors contribute to this effect. One is the gettering process which causes a steep concentration gradient to the left of the front, and a very flat gradient to the right (fig. 2). The other factors, the oxygen distribution coefficient from figure 1 and the assumption of a single diffusion mechanism, will be discussed further in the next section.

For $\beta = 0$ and $\gamma = 1.95\times10^5$ figure 5 gives a value of 295 for the gettering parameter $G/2(c_0 - c_\infty)\sqrt{Dt}$. After the front has penetrated 1 millimeter, the total amount of dissolved and combined oxygen in the structure is then 1.26×10^{-2} gram per square centimeter. In view of the very large value of u almost all of this oxygen is contained as HfO_2 between the liquid-solid interface ($u = 0$) and the gettering front ($u = u_g$).

While the example herein was inspired by a problem involving a lithium-filled heat pipe with finite gettered walls, the figures that were used pertain to a semi-infinite body. In this example, a value of $\beta = 0$ was determined which meant that no diffusing oxygen was found on the side of the front away from the oxygen source. In such cases the semi-infinite solution applies exactly until the gettering plane passes entirely through the material.

DISCUSSION

In the foregoing analysis and example, numerous assumptions were necessary in order to achieve a simple and understandable solution. Real physical situations can be expected to deviate considerably from this ideal situation.

The distribution of oxygen between lithium and tantalum used in the example was determined from figure 1, taken from reference 4. While figure 1 was based upon experimental determinations of the solubility of oxygen in lithium and in tantalum, thermochemical theory was used in its construction. A good experimental determination of the distribution coefficient has not been made. However, if the actual ratio was within the same range, 10^{-3} to 10^{-8}, as the theoretical value on figure 1, it might defy measurement. If the actual value of the distribution coefficient were much larger than the one determined from figure 1 for the example, the gettering front would progress at a proportionally higher rate than was calculated in the example.

The simple theoretical treatment discussed in this report would become more complex if possible ternary oxides of lithium, tantalum, and oxygen are formed. Ternary oxides are suspected as part of the corrosion process in contacts between refractory metals and alkali liquid metals (refs. 10 and 11). While they have not been observed with tantalum and lithium, there is always a possibility that they could play a role in the intergranular penetration of oxygen into the refractory metal. This could alter the distribution coefficient (fig. 1) and the diffusion coefficient (eq. (28)).

Further complexity in this ideal treatment would be introduced by the formation of Hf_2O and Hf_3O (ref. 12) in addition to the HfO_2 assumed. Furthermore, the solution of large amounts of oxygen in hafnium (refs. 12 and 13) could cause additional problems. Whether this can occur when the hafnium itself is a minority constituent of a solid solution is problematical. The present analysis could possibly be modified to incorporate the additional gettering implied by solution of oxygen in hafnium and the formation of lower oxides.

The assumption of local chemical equilibrium at the gettering plane led to equation (7). Although in some cases the gettering front might move so rapidly as to invalidate such an assumption, in the example just considered, the front moved very slowly after a small penetration and local chemical equilibrium was justified.

CONCLUDING REMARKS

The diffusion of oxygen into, or out of, a gettered alloy exposed to oxygenated liquid metal coolant was analyzed. Such a situation arises in heat transfer systems having gettered refractory alloy tubing with alkali liquid metal coolant.

In the analysis, the relation between the diffusion process and the theoretical thermochemistry of oxygen in the alloy and in the alkali metal was developed. Certain assumptions such as the semi-infinite extent of the alloy metal wall were necessary to achieve a simple solution. For these reasons the treatment is largely theoretical in nature.

The use of the figures developed in the analysis was illustrated by an example for oxygenated lithium coming in contact with T-111, a gettered tantalum-based alloy, at high temperature. This situation may be encountered in the startup of some heat pipes for high-temperature applications, which have been proposed and tested.

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National Aeronautics and Space Administration,
Cleveland, Ohio, March 12, 1973,
503-25.

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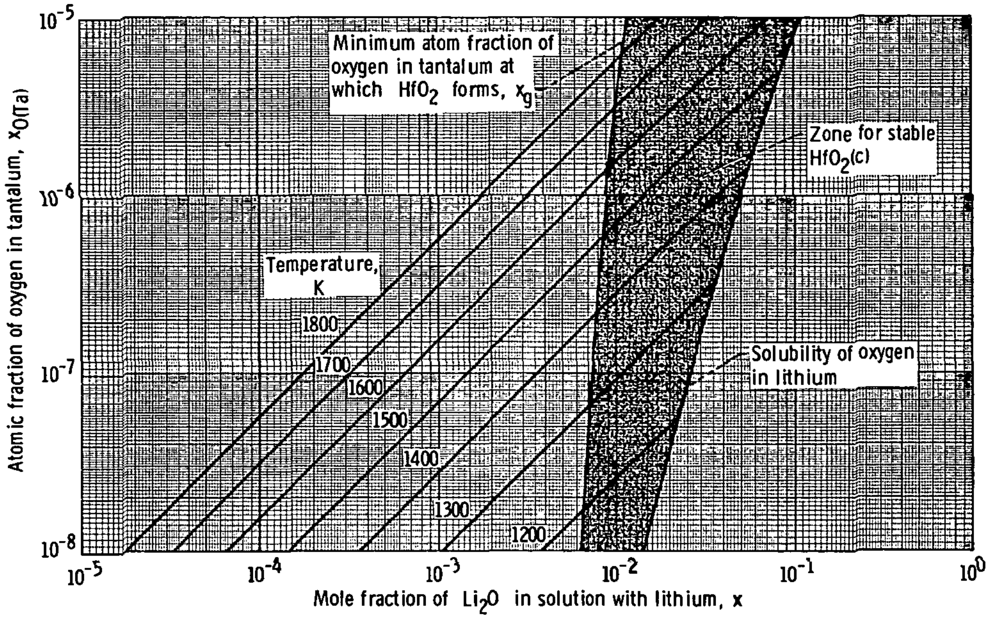
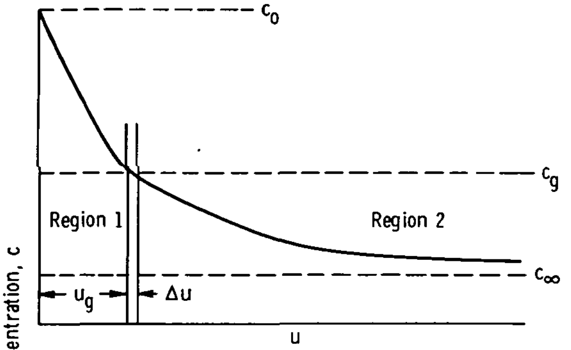
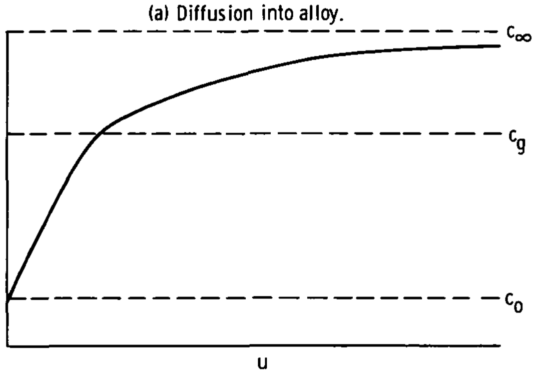


Figure 1. - Equilibrium distribution of oxygen between liquid lithium and solid tantalum at several temperatures with zone for stable $HfO_2(c)$.

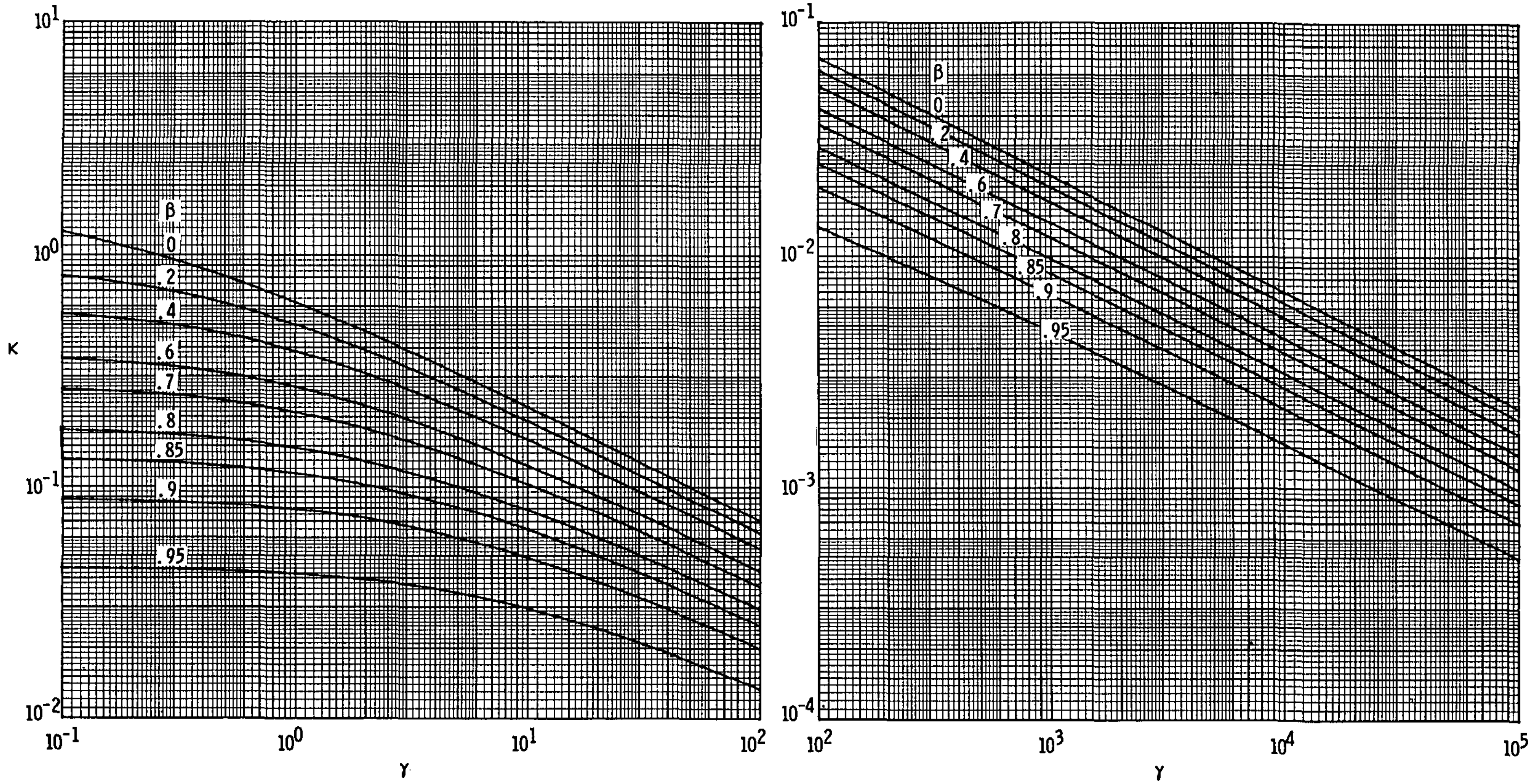


(a) Diffusion into alloy.



(b) Diffusion out of alloy.

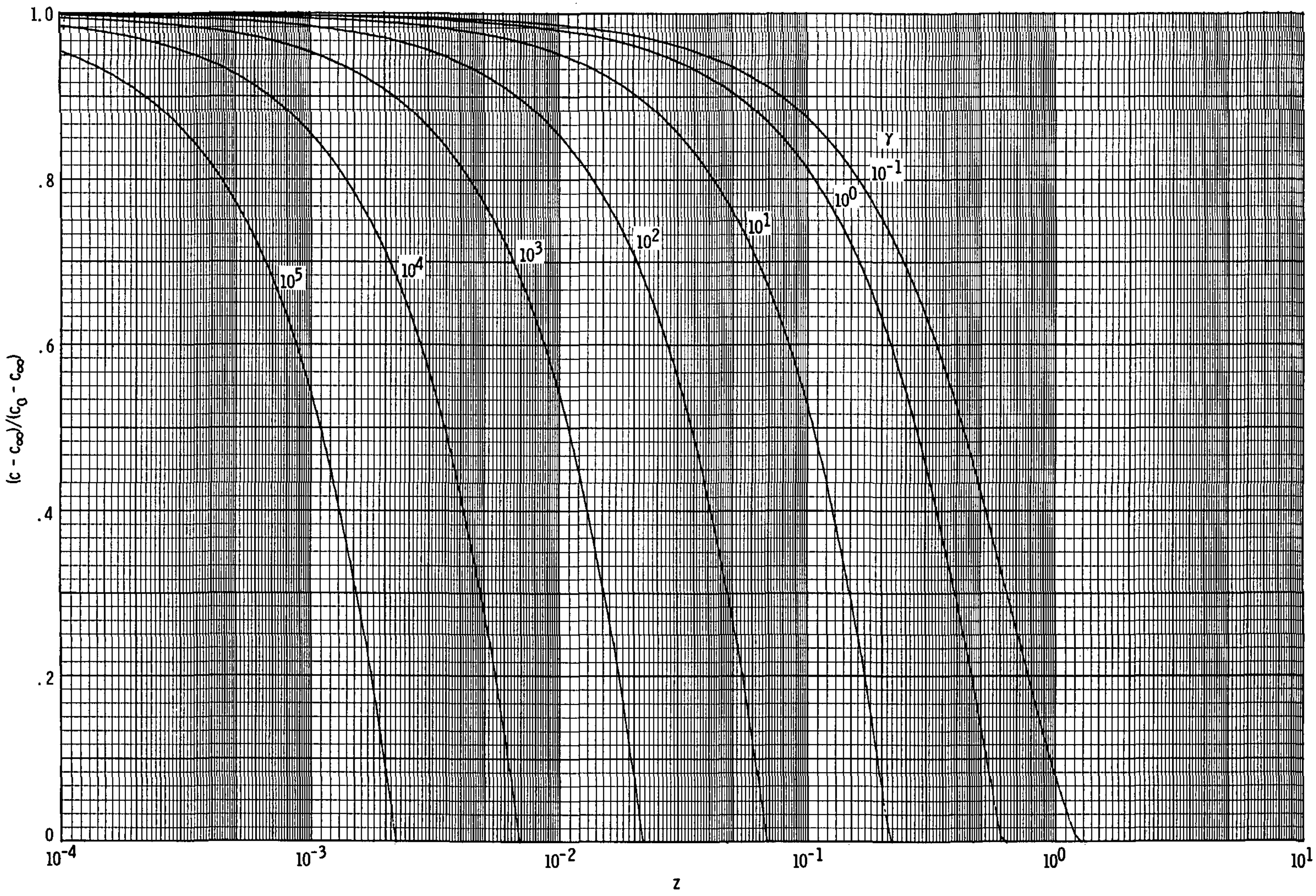
Figure 2. - Schematic illustration of oxygen diffusion into and out of semi-infinite section of gettered alloy.



(a) Range of γ, 10^{-1} to 10^{2}.

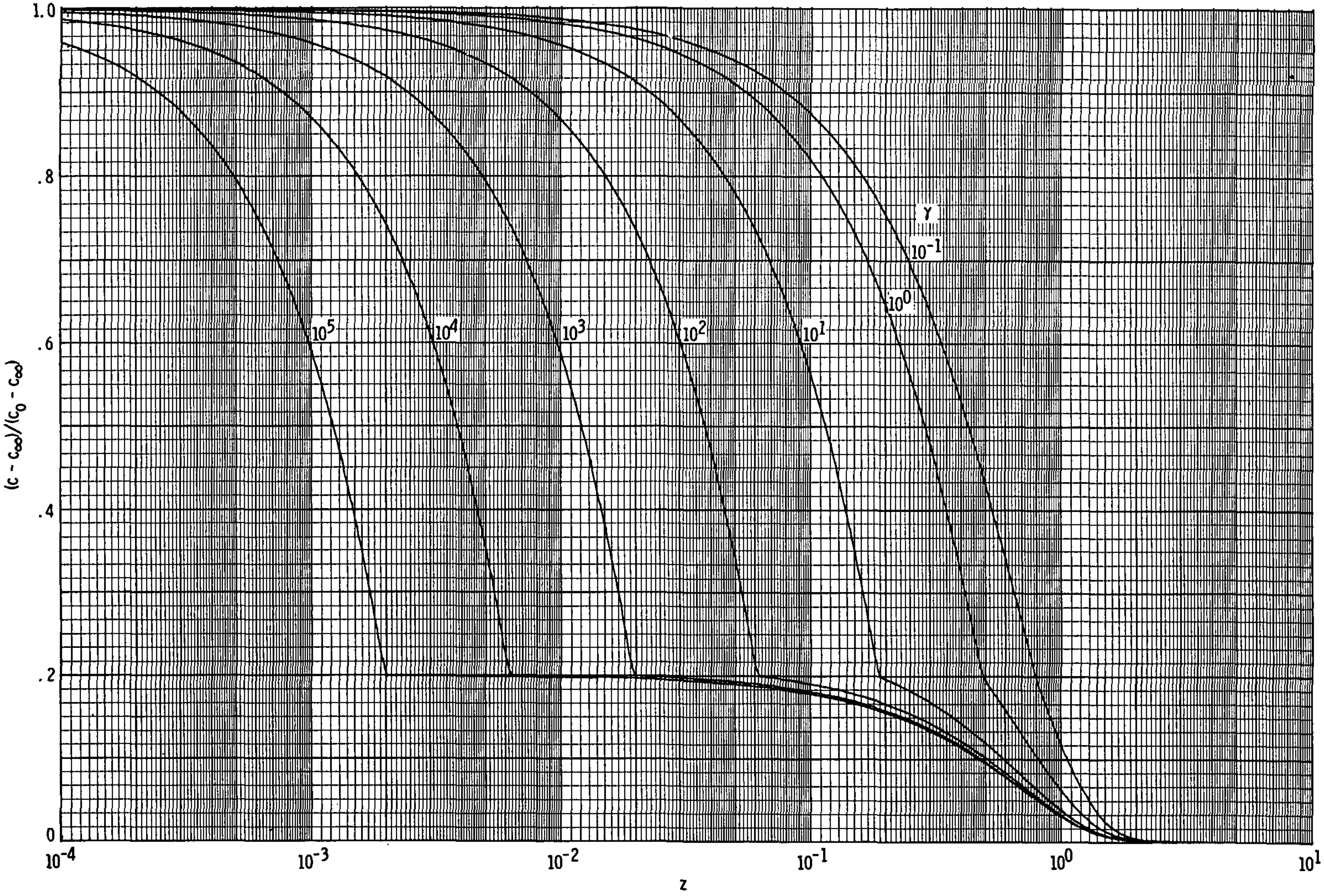
(b) Range of γ. 10^{2} to 10^{5}.

Figure 3. - Gettering plane position parameter κ slotted against γ for several values of β.



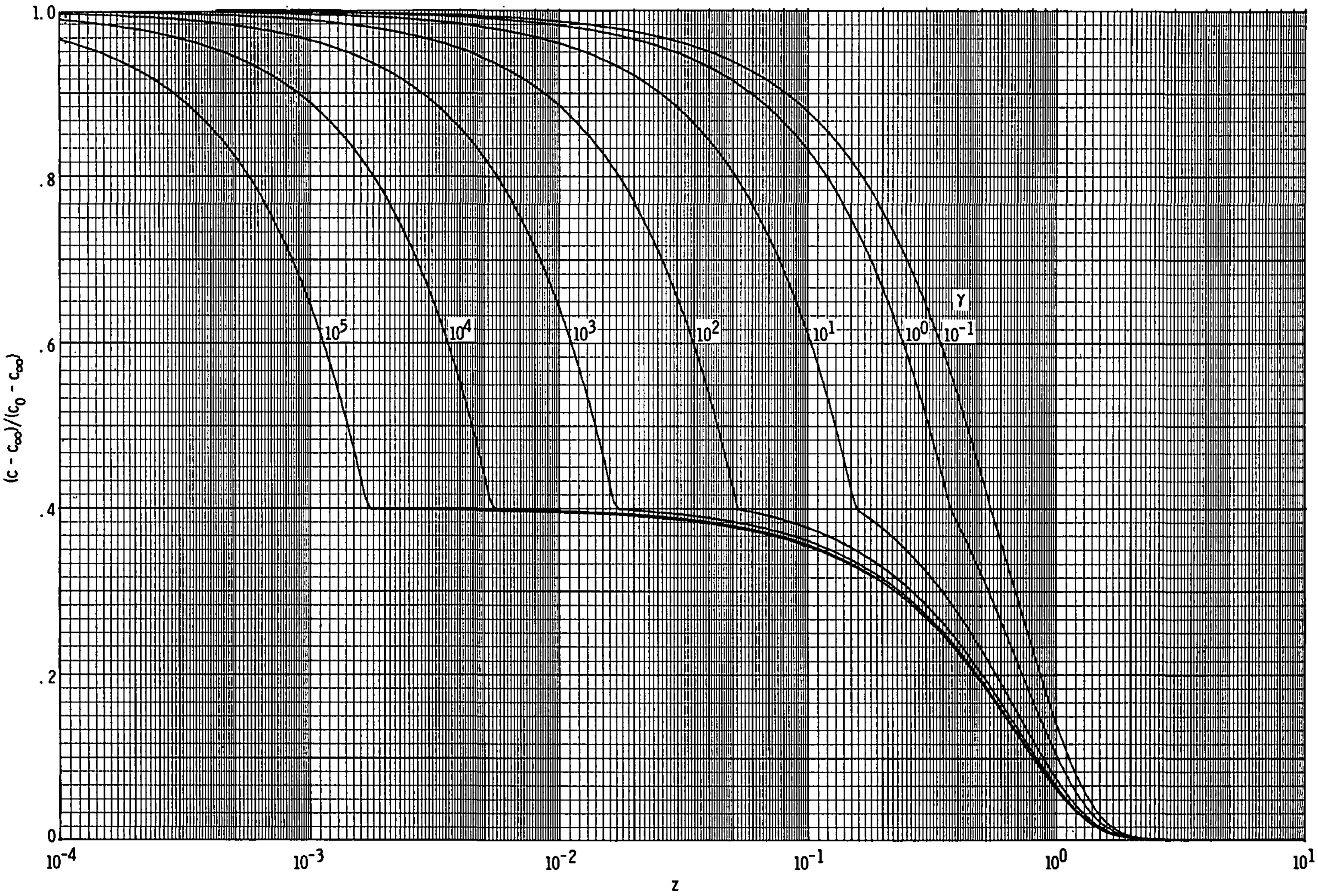
(a) $\beta = 0$.

Figure 4. - Variation of concentration function $(c - c_\infty)/(c_0 - c_\infty)$ with $z = u/2\sqrt{Dt}$ for several values of γ.



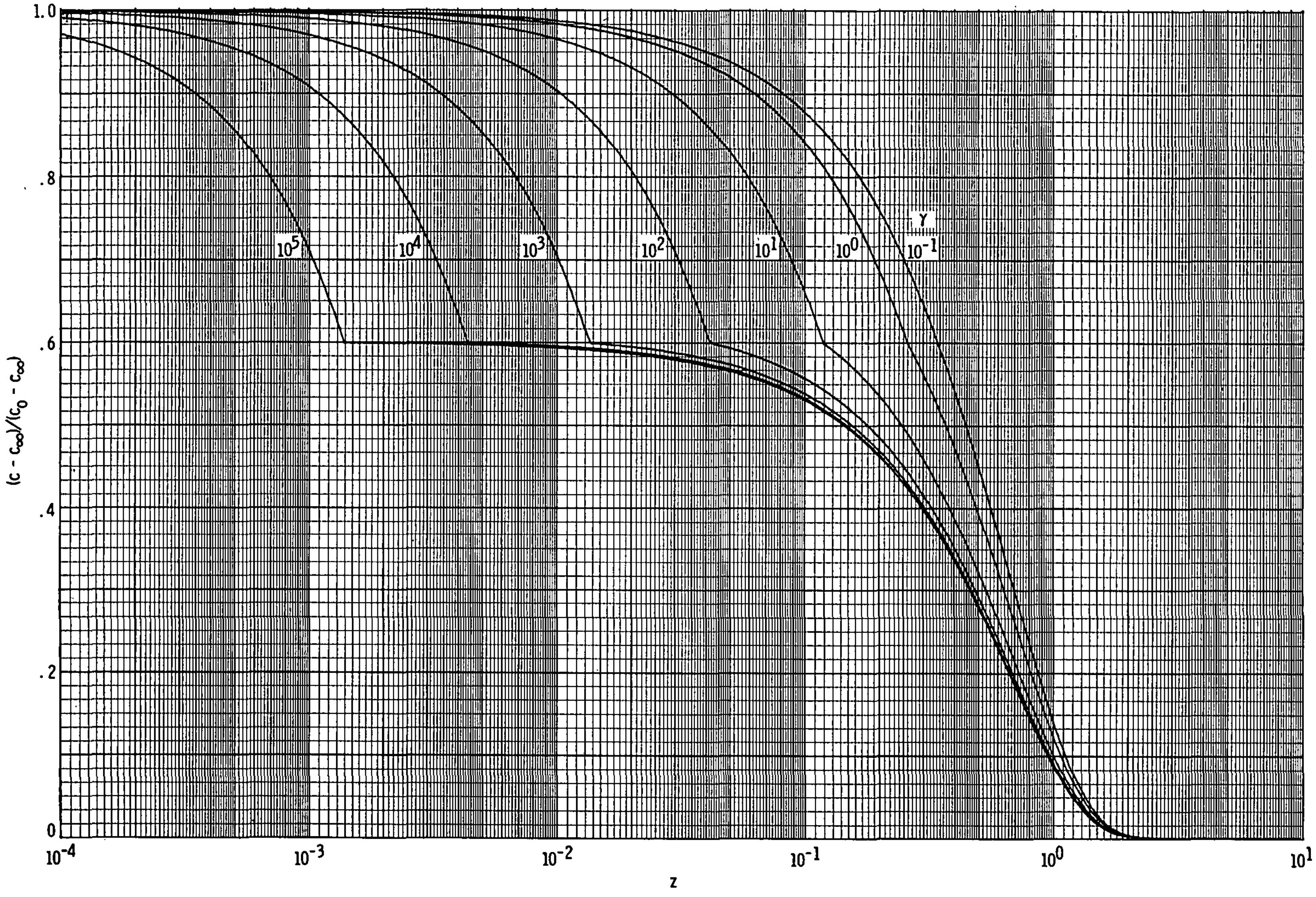
(b) $\beta = 0.2$.

Figure 4. - Continued.



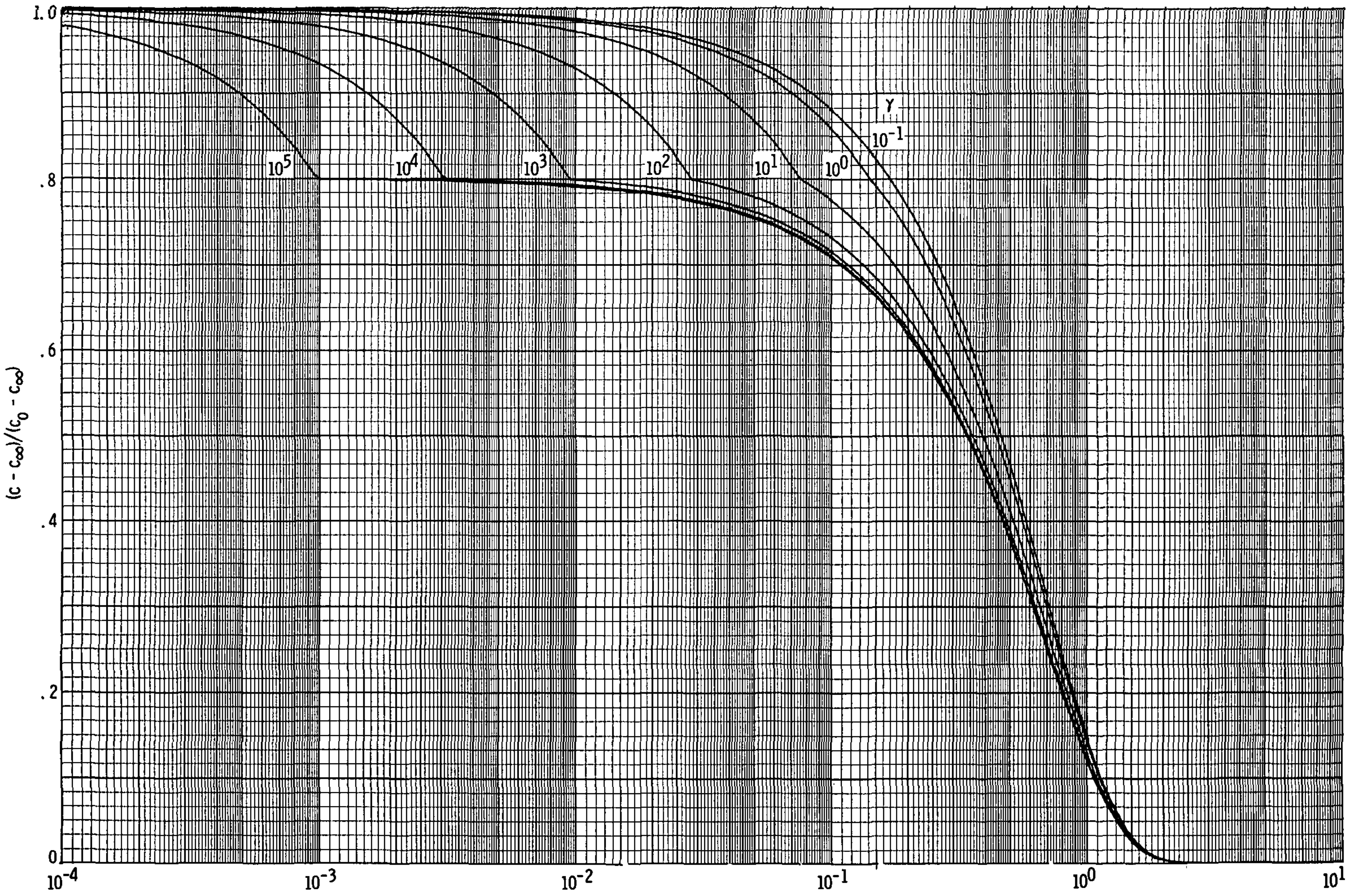
(c) $\beta = 0.4$.

Figure 4. - Continued.



(d) $\beta = 0.6$.

Figure 4. - Continued.



(e) $\beta = 0.8$.

Figure 4. - Concluded.

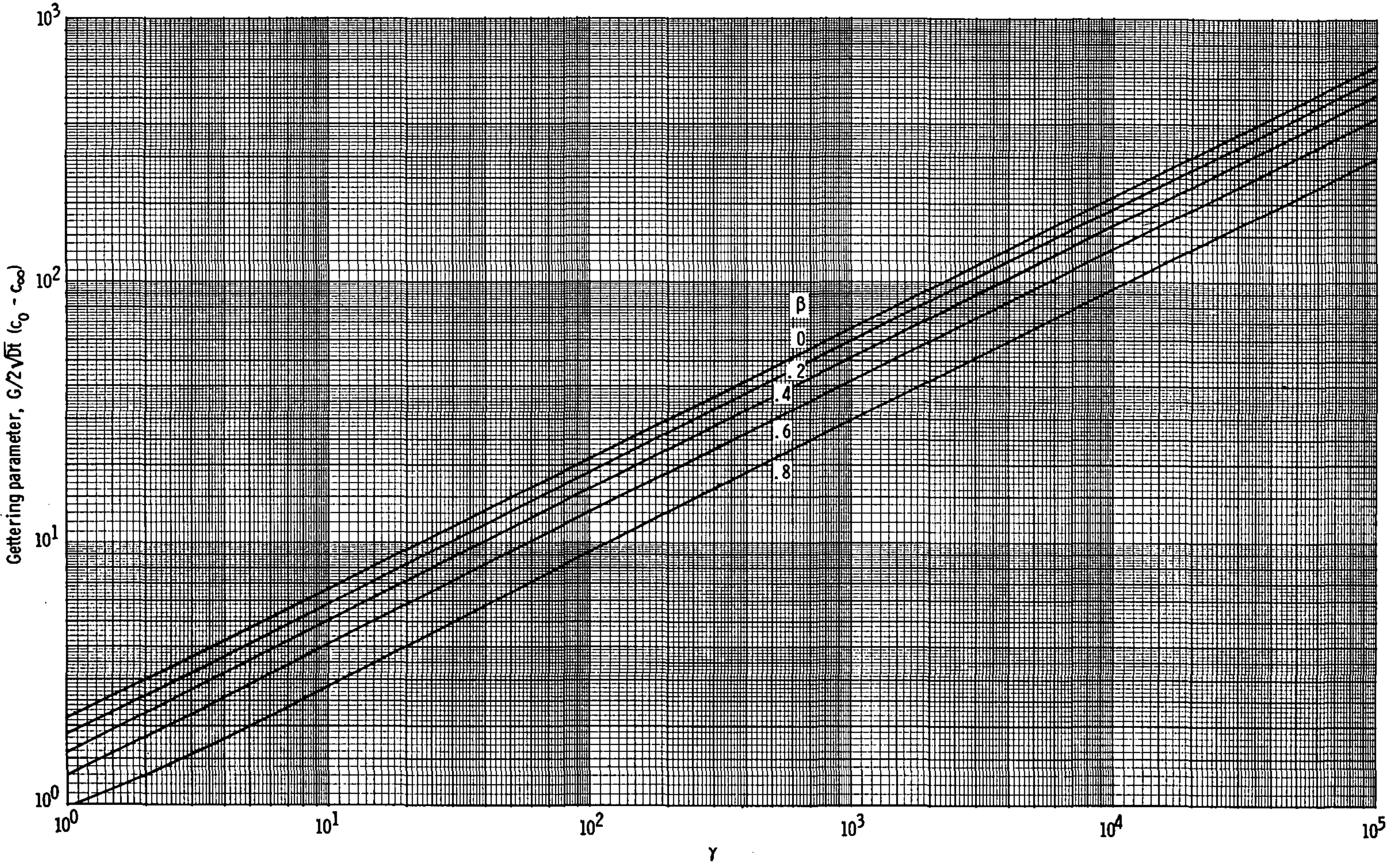


Figure 5. - Gettering parameter $G/2\sqrt{Dt}\ (c_0 - c_\infty)$ plotted against γ for several values of β.

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