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**PREDICTION OF LONG TERM CREVICE CORROSION AND HYDROGEN EMBRITTLEMENT
BEHAVIOR OF ASTM GRADE-12 TITANIUM***

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ABSTRACT

Crevice corrosion and hydrogen embrittlement are potential failure modes of Grade-12 titanium high-level nuclear waste containers emplaced in rock salt repositories. A method is presented to estimate the environment domains for which immunity to these failure modes will exist for periods of hundreds of years. The estimation is based on the identification and quantification of mechanisms involved. Macroscopic concentration cell formation is responsible for crevice corrosion. The cell formation is accompanied by oxygen depletion, potential drop, anion accumulation and acidification inside the crevice. This process is quantified by simple mass balance equations which show that the immunity domain is a function of the time the container is exposed to the corrosion environment. Strain induced hydride formation is responsible for hydrogen assisted crack initiation. A simple model for slow crack growth is developed using data on growth rates measured at various temperatures. The parameters obtained in the model are used to estimate the threshold stress intensity and hydrogen solubility limit in the alloy at infinite container service time. This value gives a crack size below which container failure will not occur for a given applied stress and hydrogen concentration, and a hydrogen concentration limit at a given stress intensity.

MASTER

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1. INTRODUCTION

A major criterion specified by the Nuclear Regulatory Commission for a high level nuclear waste package is an initial period during which radionuclide containment for 300-1000 years is required.¹ This will allow fission products to decay to low values. The main component of the waste package expected to be used in meeting this criterion is the container which will be exposed to deep geologic repository conditions. A major difficulty in nuclear waste isolation lies in demonstrating that metallic containers can resist penetration by corrosion for hundreds of years. In this paper we present a method to extrapolate experimental data to such long times.

Earlier screening tests have led to the selection of ASTM Grade-12 titanium (Ti-0.3 Mo-0.8 α , trade name of TiCode-12) as a candidate material for the container in rock salt repositories. At an assumed repository temperature of 150°C,^{3,4} various types of corrosion failure have been studied⁵ including uniform corrosion, crevice corrosion, pitting corrosion, stress corrosion and hydrogen embrittlement. Significant crevice corrosion and hydrogen embrittlement effects were detected. These two potential container failure modes have been studied extensively to identify governing mechanisms.^{6,7} Based on the identified mechanisms, models are developed and tested using experimental data. Unknown variables in the model have been estimated using these data. The models developed are used to obtain failure immunity domains for periods of hundreds of years. In this paper we emphasize the extrapolation method itself rather than give a detailed description of the physical mechanisms involved.

2. CREVICE CORROSION

Immersion tests, surface analyses and electrochemical studies have shown that macroscopic concentration cell formation is responsible for Grade-12 titanium crevice corrosion in a simulated rock salt brine at 150°C.^{5,6} The composition of the simulated rock salt brine is given in Table 1. Cell formation is accompanied by oxygen depletion, potential drop, anion accumulation and acidification inside the crevice. This leads to passivity breakdown and subsequent fast alloy dissolution. To quantify the crevice corrosion process, the anode and cathode reactions have been studied using a specially designed cell in which the two electrodes are physically separated.⁸ The anode potential, current flow from cathode to anode and pH inside the crevice are monitored.⁸

Using the measured current and maximum potential, the potential and pH drops are calculated using a simplified model for crevice corrosion. A typical example of potential change before passivity breakdown is shown in Figure 1. The anode potential is increased during the early stage of immersion because of the growth of a barrier oxide (anatase TiO₂).^{5,6} After the maximum potential is reached, non-barrier oxide (rutile TiO₂) forms and the following three types of potential change are dominant: (1) potential drop caused by oxygen concentration change,⁹ (2) Ohmic potential drop,¹⁰ (3)

potential rise due to excess proton generation¹¹ (Junction Potential). These are less important before the maximum potential is obtained.

The anode potential rise during the growth of barrier oxide is given by the following mass balance relationship:

$$V(\text{oxide}) = V_i + \frac{I_p t M}{C \rho F} \quad (1)$$

where ρ is the density of the anatase form of TiO_2 , V_i is the initial reference potential, C is a system constant,¹² I_p is the passive current estimated from the maximum potential observed, t is the time, M is the molecular weight of TiO_2 , and F is the Faraday constant. The potential drop due to oxygen concentration changes may be approximated by the Nernst equation assuming a constant exchange current.⁹

$$V(\text{O}_2) = V_i + \frac{RT}{F} \ln \left(\frac{C(\text{O}_2)}{C_i(\text{O}_2)} \right) \quad (2)$$

where $C_i(\text{O}_2)$ is the initial oxygen concentration and $C(\text{O}_2)$ is the oxygen concentration at time t . $C(\text{O}_2)$ is obtained by a simplified diffusion equation:

$$C(\text{O}_2) = C_i(\text{O}_2) - \frac{2 I_p t}{H F} + \frac{2 D_{\text{O}_2} t}{x \delta} [C_i(\text{O}_2) - C(\text{O}_2)] \quad (3)$$

where x is the crevice depth, H is the crevice gap size, δ is the effective distance of oxygen concentration gradient within the crevice and D_{O_2} is the oxygen diffusivity. The second term represents oxygen consumption and the third term represents oxygen diffusion inflow. Upon separation of the anode and cathode areas, a current I flows from the cathode to the anode resulting in the accumulation of protons and in the migration of anions to the crevice. Since the diffusivities of minor anions are smaller than that for chloride,¹³ only chloride ion migration is considered here. The accumulated concentrations of protons $C(\text{H}^+)$ and chloride $C(\text{Cl}^-)$ are given by the following mass balance equations:^{14,15,16}

$$C(\text{H}^+) = C_i(\text{H}^+) + \frac{2 I t}{F H} - \frac{2 D_{\text{H}^+} t}{x \delta} [C(\text{H}^+) - C_i(\text{H}^+)] - \frac{2 C(\text{H}^+) D_{\text{H}^+} t F}{x R T} \left(\frac{q}{\epsilon \delta^2} \right) \quad (4)$$

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$$C(\text{Cl}^-) = C_1(\text{Cl}^-) + \frac{2 D_{\text{Cl}^-} t}{x \delta} [C(\text{Cl}^-) - C_1(\text{Cl}^-)] + \frac{2 C_1(\text{Cl}^-) D_{\text{Cl}^-} t F}{x R T} \left(\frac{1}{\epsilon \delta^2} \right) \quad (5)$$

where $C_1(\text{H}^+)$ and $C_1(\text{Cl}^-)$ are initial concentrations of proton and chloride, respectively, and D_{H^+} and D_{Cl^-} are diffusivities of protons and the chloride, respectively. ϵ is the dielectric constant and q is the excess charge inside the crevice. The above two equations have diffusion terms arising from concentration gradient and field enhanced diffusion (migration). From these two equations, the ohmic potential drop may be given by:^{10,17}

$$V(\text{ohmic}) = V_1 + \frac{RT}{F} \ln \left[\frac{C_1(\text{HCl})}{C(\text{HCl})} \right] \quad (6)$$

where $C_1(\text{HCl})$ and $C(\text{HCl})$ are HCl concentrations at $t=0$ and t , respectively. The junction potential rise may be similarly formulated:

$$V(\text{junction}) = V_1 + \frac{\pi F x^2 H [C(\text{H}^+) - C_1(\text{H}^+) - C(\text{Cl}^-) + C_1(\text{Cl}^-)]}{\epsilon \delta} \quad (7)$$

In the calculation at 150°C, I values have been obtained from experiments and q values have been adjusted. The temperature dependencies of I and q are obtained from the literature²¹. Because of the limited data available, I and q have been assumed to be dependent on temperature either linearly (Case 1) or exponentially (Case 2). At 150°C, the best fit is obtained with $\delta = 0.3$ cm, $q = 8.0 \times 10^{-14}$ coul (Case 1) and 8.0×10^{-15} coul (Case 2), as shown in Figure 1, resulting in the calculated pH = 3.63 and $C(\text{Cl}^-) = 190006$ ppm for (Case 1) and pH = 2.63 and $C(\text{Cl}^-) = 190063$ ppm for (Case 2) at 80 hours. The rest of the parameters used in the calculation are given in Appendix 1. The measured pH within the crevice at room temperature is two to three, which is in agreement with calculated values. Also, because the brine solution has a near saturated Cl^- ion concentration, the calculated Cl^- concentration may be a realistic value because $C(\text{Cl}^-)$ greater than the initial value of 190000 ppm may produce precipitates.

For extrapolation purposes, we use $\delta = 0.3$ cm, pH = 2.63 and 3.63 and an initial value of $C(\text{Cl}^-)$ for passivity breakdown as 190,000 ppm based on the above reasoning. Using Equation (4), a map is drawn in the space of $C_1(\text{Cl}^-)$ and T ; Figure 2 is the result assuming a linear dependence of current on temperature while Table 2 is that for an exponential dependence. As shown in Figure 2, the domain for crevice corrosion is enlarged as corrosion times are increased, and eventually it reaches the threshold value, C_{th} , below which crevice corrosion does not occur even at infinite service time. Table 2 also shows such a trend even though the time dependence is relatively insignificant compared to Figure 2. Also, there will be a temperature limit,

T_{th} , below which mass flow ceases. Since the calculated T_{th} is close to absolute zero, the actual T_{th} may be close to the brine freezing point, which is contrary to the basic assumptions involved. The dotted line in Figure 2 represents such uncertainties. The domain obtained here (Figure 2 and Table 2) has been verified experimentally before.¹⁸

3. HYDROGEN EMBRITTLEMENT

Notched and unnotched specimens of hydrogenated Grade-12 titanium have been mechanically tested in tension at room temperature. For as-received hydrogen levels (35 ppm) and greater, internal hydrogen embrittlement is present.⁷ A comparison of fractographs with those in other alpha-beta alloys leads to the conclusion that hydride formation is responsible for the hydrogen embrittlement.⁷ To quantify the results, slow crack growth rates have been measured at various temperatures. The measured activation energy for crack growth is lower than the activation energy for hydrogen diffusion in the alpha phase matrix. Also, there is a maximum temperature above which crack growth rates are lowered. We have modified a crack growth kinetics model by incorporating dislocation pipe hydrogen diffusion and hydride nucleation kinetics to quantify the role of internal hydrogen embrittlement in the crack propagation process.

For hydrogen-diffusion-controlled crack propagation, the stage II crack growth rates may be given by:^{5,23}

$$\frac{da}{dt} = \frac{2}{C_Y^e} \frac{k_1}{1 - k_2/f} \quad (8)$$

where

$$k_1 = 2 \pi D_H C_O L b^2 \exp\left(\frac{E_B}{kT}\right) \exp\left(\frac{P\bar{V}_H}{kT}\right)$$

$$k_2 = \frac{D_H}{k T} \left(\frac{dP}{dx}\right) - \frac{2 D_H}{d}$$

$$f = \frac{\pi d}{2 l} \left(\frac{D_H}{t_H}\right)^{1/2} L b^2 \exp\left(\frac{E_B}{kT}\right)$$

where

$$P = \frac{r \sigma_y}{d} [(1+2 d/r) \ln(1+2 d/r) - (1+d/r) \ln(1+d/r) - 0.5 d/r]$$

$$\frac{dP}{dx} = \frac{\sigma_y}{d} [\ln(1+2 d/r) - \ln(1+d/r) + 0.5]$$

where

$$r = K^2 / (\sigma_y E_y)$$

where K is the stress intensity, E_y is Young's modulus, D_H is the hydrogen pipe diffusivity in alpha phase, C_0 is the hydrogen concentration at alpha phase adjacent to beta phase, L is the dislocation density in the plastic zone around the crack tip, b is Burger's vector, E_B is the binding energy of hydrogen to a dislocation, σ_y is the yield strength, l is the hydride size, t_H is the crack jump time, V_H is the partial molar volume of hydrogen in titanium. C_Y^e is the hydrogen concentration in the hydride phase, and d is average grain size.

For stage II crack propagation which is controlled by hydride nucleation at the crack tip, the relationship is:^{5,23}

$$\frac{da}{dt} = 0.5 \pi l^3 d C_Y^e C_0 L b^2 \left(\frac{kT}{h}\right) \exp\left(\frac{E_B}{kT}\right) \exp\left(\frac{-\Delta G^*}{kT}\right) \exp\left(\frac{-\Delta G_d}{kT}\right) \quad (9)$$

where ΔG^* is the activation energy for hydride nucleation on dislocations (see Appendix 2) and ΔG_d is the activation energy for dislocation pipe hydrogen diffusion.

In the regime of the threshold stress intensity (K_{th}), the crack growth mode is stage I. To obtain K_{th} , a solubility limit consideration is adopted for stage I. The hydrogen solubility in the presence of hydride and applied stress is given²⁴ by:

$$C_E = \exp[(-\Delta G^0 + P_E V_H - W_p - E_{KK} \bar{V}_H P_E) / kT] \quad (10)$$

$$P_E = \frac{4(1+\nu)K}{3(2\pi)^{1/2} d^{1/2}} \quad (11)$$

where ΔG^0 is the free energy of hydride formation, ν is Poisson's ratio, W_p is plastic work done during hydride formation by dislocation movement, E_{KK} is the stress free transformation strain, $\bar{V}_H$ is the partial molar volume of hydrogen in hydride. The concentration of hydrogen due to external stress is given by:²⁴

$$C_H = C_0 \exp(P_E \bar{V}_H / kT) \quad (12)$$

Equating Equation (10) and Equation (12) gives the threshold stress intensity values. The K values have been varied above the K_{th} values until the incubation time^{5,24} for nucleation kinetics of Equation (9) would be negligible. This enables us to determine true K_{th} at infinite time.

Figure 3 shows experimental crack growth rates for $K = 60-80 \text{ MPa } \sqrt{\text{m}}$ at various temperatures. Figure 4 gives the calculated values rate controlled by hydrogen pipe diffusion (diffusion kinetics) ($L = 10^9/\text{cm}^2$, $E_B = 0.35 \text{ eV}$, $t_H = 1 \text{ sec}$, $Q = 0.65, 0.70, 0.75 \text{ and } 0.80$). Q is the ratio of activation energy of pipe diffusion to that of lattice diffusion. Figure 5 shows diffusion kinetics (solid line at $L = 10^{11}/\text{cm}^2$, $E_B = 0.25 \text{ eV}$, $t_H = 1 \text{ sec}$, $Q = 0.70 \text{ and } 0.80$). Nucleation kinetics are evaluated (triangles) at 90°C and 120°C . At 90°C , $\alpha = 0.6$ and $\sigma = 67 \text{ erg/cm}^2$ are used while $\alpha = 0.3$ and $\sigma = 85 \text{ erg/cm}^2$ are used. The rest of the parameters are in Appendix 2. Figure 4 shows the decrease in the crack growth rates at higher temperature regimes while Figure 5 shows a sharp drop from solid line to triangles either at 90°C or at 120°C which are chosen for comparison.

The threshold stress intensity, K_{th} is obtained from Equation (10) and Equation (12). At 150°C and $C_0 = 35 \text{ ppm}$ with hydrogen accumulation factor 2 of alpha phase adjacent to beta phase,^{25,26} the K_{th} value is $4.86 \text{ MPa } \sqrt{\text{m}}$. At and below $K = K_{th}$, the incubation time^{5,23} for hydride nucleation is infinity using parameters in the calculation of Figure 4. Also, if K is increased to K_{th} plus maximum a $2 \times 10^{-6}\%$ of K_{th} , the incubation time is reduced to be 85-250 seconds within the parameter variations used in Figure 4. Therefore, we may conclude that the container will not fail when it is subjected to a stress intensity below $4.86 \text{ MPa } \sqrt{\text{m}}$ at 150°C and initial hydrogen concentration of 35 ppm for very extended time periods. Table 3 shows an estimated minimum crack size allowed from the K_{th} values at various applied stress levels. It is seen that crack sizes less than 0.29 mm can cause failure at and above stress level of the half of yield strength. Table 4 is an estimated minimum hydrogen concentration at 150°C to avoid failure at various stress intensity levels using the same parameters. At a given stress intensity, when the hydrogen levels are below the value in Table 4, the delayed failure will be avoided according to this calculation.

4. DISCUSSION

In the crevice corrosion evaluation, δ and q are adjustable parameters. δ alone, nevertheless, is partly verified by experimental observation. Severe crevice corrosion at the edge of the specimen supports the δ value is very small compared to the specimen size.⁸ This is true in our calculation. Numerically q value depends on the Δt we choose, which gives a huge unrealistic excess charge if Δt is too great. Therefore, we have chosen q as an adjustable parameter and the extracted values from potential drop are found to be reasonable.

In the hydrogen embrittlement, there is ample evidence that $L \leq 10^{11}/\text{cm}^2$,²⁷ $0.1 \leq E_B \leq 0.5 \text{ eV}$,²⁸ $10 \leq \sigma \leq 1000$ ²⁹ erg/cm^2 . α and Q are fractions of those in the lattice and are known to be less than unity.^{30,31} The rest of the parameters quoted in the Appendix are from either CP titanium or near alpha-beta titanium alloys or Grade-12 titanium. Since alpha phase is depleted of alloying elements, these parameters are not unrealistic.

We have not considered the temperature variations in the repository over extended periods. However, the estimation of the crevice corrosion behavior at 150°C is probably applicable as a conservative analysis of performance at lower temperatures for more extended periods, since it is generally accepted that the crevice corrosion mechanism does not change at a temperature variation from boiling point to room temperature.³² Our hydrogen embrittlement data are based on temperature variations to room temperature. Therefore, estimation of behavior at lower temperatures than 150°C is feasible. Dynamic estimation with temperature variation during test may need enormous efforts if carried out.

5. CONCLUSION

In the current study we have outlined a method for estimating very long term crevice corrosion and hydrogen embrittlement behavior of Grade-12 titanium in high temperature brine. Full details of the physical and chemical mechanisms involved were not given since the objective of this paper is to explain the basis for the extrapolation of short term data to very extended times of hundreds of years. An important feature in this study is that the kinetics parameters (particularly corrosion time) have been incorporated in thermodynamics and mechanics parameters. This enables us to extrapolate the results to extended periods.

In the models developed, values for several parameters are not known and some have been estimated from known values of similar materials. In other cases, estimates had to be made and the values were selected to maintain internal consistency within the calculations. If direct measurements of the parameters had been performed, the accuracy of the calculation would have been improved.

A full description of the individual measurement involved in the crevice corrosion and hydrogen embrittlement processes is given elsewhere.⁵

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Table 1. Composition of a simulated rock salt brine.

Component	Na ⁺	K ⁺	Mg ⁺²	Ca ⁺²	Sr ⁺²	Cl ⁻	SO ₄ ⁻²	I ⁻	HCO ₃ ⁻	Br ⁻	BO ₃ ⁻³
Concentration (ppm)	42,000	30,000	35,000	600	5	190,000	3,500	10	700	400	1,200

Table 2. Initial Cl⁻ concentration (ppm) necessary for passivity breakdown in Grade-12 titanium crevice corrosion at various times and 150°C in a simulated rock salt brine. The current is assumed to be exponentially dependent on temperature. The critical anion concentration used is 190000 ppm.

T (°C)	t = 5 h	t = 150 h	t = 1000 h	t = ∞
80	189242	189023	189014	189013
100	181477	179825	179766	179756
120	133729	128062	127879	127846
140	47377	43693	43582	43562
160	10108	9341	9319	9315
180	2103	1969	1966	1965
200	487	461	461	460
220	127	121	121	121
240	37	35	35	35
260	12	11	11	11
280	4	4	4	4
300	2	1	1	1

Table 3. Estimated minimum safe flaw size of as-received Grade-12 titanium at various applied stresses (temperature 150°C).

Stress, σ	YS	0.5 YS	0.1 YS	0.05 YS	0.01 YS
Crack size, a (mm)	0.07	0.29	7.3	28.7	731.0

Yield Strength (YS) (at 150°C) = 320.6 MPa, $K_{th} = 4.86 \text{ MPa } \sqrt{\text{m}}$
 The calculation is based on $K_{th} = \sigma \sqrt{\pi a}$

Table 4. Hydrogen concentration allowed in alpha phase for safe performance of as-received Grade-12 titanium at various applied stress intensities (temperature 150°C).

Stress intensity (MPa $\sqrt{\text{m}}$)	K	0.4	1.2	3.9	12.3	38.7	122.5
Hydrogen concentration (ppm)	C	42.2	40.7	36.4	25.4	8.2	0.2

- Figure 1. Measured (circles) and calculated (solid line) potentials at various times in the Grade-12 titanium crevice corrosion in a simulated rock salt brine at 150°C.
- Figure 2. Immunity domains in temperature and initial anion concentration necessary for passivity breakdown at various service times for Grade-12 titanium in a simulated rock salt brine. The current is assumed to be dependent on temperature linearly. The critical anion concentration used for passivity breakdown is 190000 ppm.
- Figure 3. The measured slow crack growth rates of as-received Grade-12 titanium for $K = 60$ to $80 \text{ MPa} \sqrt{\text{m}}$ at various temperatures.
- Figure 4. The calculated slow crack growth rates of as-received Grade-12 titanium controlled by hydrogen pipe diffusion for all K values at various temperatures. Q factor is a ratio of activation energy of pipe diffusion to that of lattice diffusion.
- Figure 5. The calculated hydrogen pipe diffusion kinetics plus nucleation kinetics (triangles). For nucleation control, four triangles are from $K = 42, 56, 80, 127 \text{ MPa} \sqrt{\text{m}}$ at 120°C and three triangles are from 42, 56, 80 $\text{MPa} \sqrt{\text{m}}$ at 90°C. Open triangles are for $Q = 0.70$ and solid triangles are for $Q = 0.80$.

Figure 1. Measured (circles) and calculated (solid line) potentials at various times in the Grade-12 titanium crevice corrosion in a simulated rock salt brine at 150°C.

Figure 2. Immunity domains in temperature and initial anion concentration necessary for passivity breakdown at various service times for Grade-12 titanium in a simulated rock salt brine. The current is assumed to be dependent on temperature linearly. The critical anion concentration used for passivity breakdown is 190000 ppm.

Figure 3. The measured slow crack growth rates of as-received Grade-12 titanium for $K = 60$ to $80 \text{ MPa}\sqrt{\text{m}}$ at various temperatures.

Figure 4. The calculated slow crack growth rates of as-received Grade-12 titanium controlled by hydrogen pipe diffusion for all K values at various temperatures. Q factor is a ratio of activation energy of pipe diffusion to that of lattice diffusion.

Figure 5. The calculated hydrogen pipe diffusion kinetics plus nucleation kinetics (triangles). For nucleation control, four triangles are from $K = 42, 56, 80, 127 \text{ MPa}\sqrt{\text{m}}$ at 120°C and three triangles are from $42, 56, 80 \text{ MPa}\sqrt{\text{m}}$ at 90°C . Open triangles are for $Q = 0.70$ and solid triangles are for $Q = 0.80$.

APPENDIX 1

PARAMETERS USED IN THE CALCULATION OF CREVICE CORROSION

δ = 0.3 cm (adjustable, but upper limit is confirmed by experiment)

ρ = 3.84^{19}

H = 2 μ m (experimental value)

ϵ = 50 ϵ_0^{11}

D_{O_2} = $0.0821 \exp(-2440/T)^{20}$

D_{H^+} = $\exp(-1700/T)^{20}$

C_{Cl^-} = $0.0508 \exp(-2327/T)^{20}$

Case 1: $I = 8.3 \times 10^9 \exp(-16095/T)^{21,22}$ coulomb/cm²-sec
 $q = 2.7 \times 10^2 \exp(-16095/T)$ coulomb (adjustable parameter)

Case 2: $I = 5.84 \times 10^{-10} T^{21}$ coulomb/cm²-sec
 $q = 1.89 \times 10^{-16} T$ coulomb (adjustable parameter).

APPENDIX 2

PARAMETERS USED IN THE CALCULATION OF HYDROGEN EMBRITTLEMENT

C_Y^e	=	0.6580 ¹⁹		
C_o	=	35 ppm is the average initial hydrogen concentration. There will be an enrichment factor near the beta phase ^{25,26} (a factor of 2 is used).		
L	=	$10^9/\text{cm}^2$ (Figure 3), $10^{11}/\text{cm}^2$ (Figure 4)		
B	=	0.59 nm ³³		
E_B	=	0.35 eV (Figure 3), 0.25 eV (Figure 4) ²⁸		
$\bar{V}_H$	=	1.68 cm ³ /mole ²⁴		
$\bar{V}_h$	=	12.50 cm ³ /mole ²⁴		
d	=	2 μ (experimental)		
l	=	0.67 μ (experimental)		
t_H	=	1 sec (adjustable)		
E_y	=	110.3 MPa ²⁸	σ_y (20°C)	= 538 MPa ³⁶
ΔG^o	=	18.6 KJ/mol ³⁴	σ_y (40°C)	= 400 MPa
W_P	=	0.67 KJ/mol ²⁰	σ_y (60°C)	= 386 MPa
E_{KK}	=	0.24 ²⁰	σ_y (80°C)	= 372 MPa
	=	0.33 ²⁸	σ_y (100°C)	= 359 MPa
D_H	=	0.06 exp(-Q 7200/T) ³⁵	σ_y (130°C)	= 334 MPa

$$\Delta G^* = \alpha 16 \pi \sigma^3 / (3 G_V^2)$$

$$\text{where } G_V = -[C_H \bar{V}_H + (1-C_H) \bar{V}_{Ti}]^{-1} / (TANT + GM + GMIN + \Delta G^o)$$

$$\begin{aligned} \text{where } TANT &\equiv R T (C_Y^e - C_H) [\ln C_H - \ln (1-C_H) + \ln (GAM)] \\ GAM &\equiv 1/C_E \exp[(1-C_E)*(-\Delta G^o)/((C_Y^e - C_E) R T)] \\ GMIN &\equiv 1/(1 + GAM) \\ GM &\equiv R T [(1-C_H) \ln (1-C_H) + C_H \ln (GAM C_H)] \end{aligned}$$

α is the ratio of nucleation barrier in dislocation to that in bulk matrix,³⁰
 σ is the interfacial energy and $\bar{V}_{Ti}$ is obtained from $\bar{V}_H$.³⁷