

**Supporting material for:**

**Thermodynamic Insights into the Henry's Constant in Silicon  
Hyperthermal Oxidation for Fabricating Optical Waveguides**

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# 1. Thermal/chemical energies and Henry's law constant in the silicon hyperthermal oxidation system:

With Equations (22)-(25) in the manuscript, we use the software tool – Matlab program and simulate the distributions of the thermodynamic and chemical reaction energies with respect to three temperature values: 700°C, 1000°C and 1300°C as shown in Figure 2(a), then with Equation (8) obtain the total internal energy of one molecule as shown Figure 2(b). Further, we simulate the Henry's constant  $H$  in the hyperthermal oxidation process of silicon with respect to these three temperature values as shown in Figure 3(a), then by setting an oxidation time of 1.0 h, we simulate the temperature dependence of  $H$  as shown in Figure 3(b). The follows are the start and end parts of the program.

```
14 INTERE_RIGHTH_SIOXIDATION_vs_TIME_01A.m INTERE_RIGHTH_SIOXIDATION_vs_TIME_01B.m
3 % This program is to calculate the INSIDE ENERGY in the Si OXIDATION
4 % The theoretical models are from the thermodynamics of gas system
5 % The difference of 01B from 01A is this 01B is for the multiple temperature
6
7 clear
8
9 % Definitions of all the parameters in the thermodynamic physics
10
11 % epsilon_x: x component of the dielectric constant vector.
12 % epsilon_y: y component of the dielectric constant vector.
13 % epsilon_s: the dielectric constant of substrate SiO2.
14 % adjust_b: adjust factor for boardary continuity
15
16 lambda_mic=1.55;
17 c=3.0e+8;
18
19 % Input values into parameters as follows:
20
21 %choice=1;
22 %choice=2;
23 %choice=3;
24 %choice=4;
25 choice=1232;

257 semilogy(tox_hr,Uthem_3,Uchem_3)
258 xlabel('Oxidation time t_o_x (hr)')
259 ylabel('Energy rate (J/min)')
260 title('Therm & Chem energy rate in Si oxidation')
261 plotedit
262 end
263
264 if choice==123
265 semilogy(tox_hr,E_inter_1,tox_hr,E_inter_2,tox_hr,E_inter_3)
266 xlabel('Oxidation time t_o_x (hr)')
267 ylabel('Interenergy rate (J/min)')
268 title('Internal energy rate in Si oxidation')
269 plotedit
270 end
271
272 if choice==1232
273 semilogy(tox_hr,Uthem_1,tox_hr,Uchem_1,tox_hr,Uthem_2,tox_hr,Uchem_2,tox_hr,Uthem_3,tox_hr,Uchem_3)
274 xlabel('Oxidation time t_o_x (hr)')
275 ylabel('Interenergy rate (J/min)')
276 title('Internal energy rate in Si oxidation')
277 plotedit
278 end
279
```

## 2. Analysis for the diffusivity effect upon the Growth rate of silicon dioxide (SiO<sub>2</sub>) in the thermodynamic mode

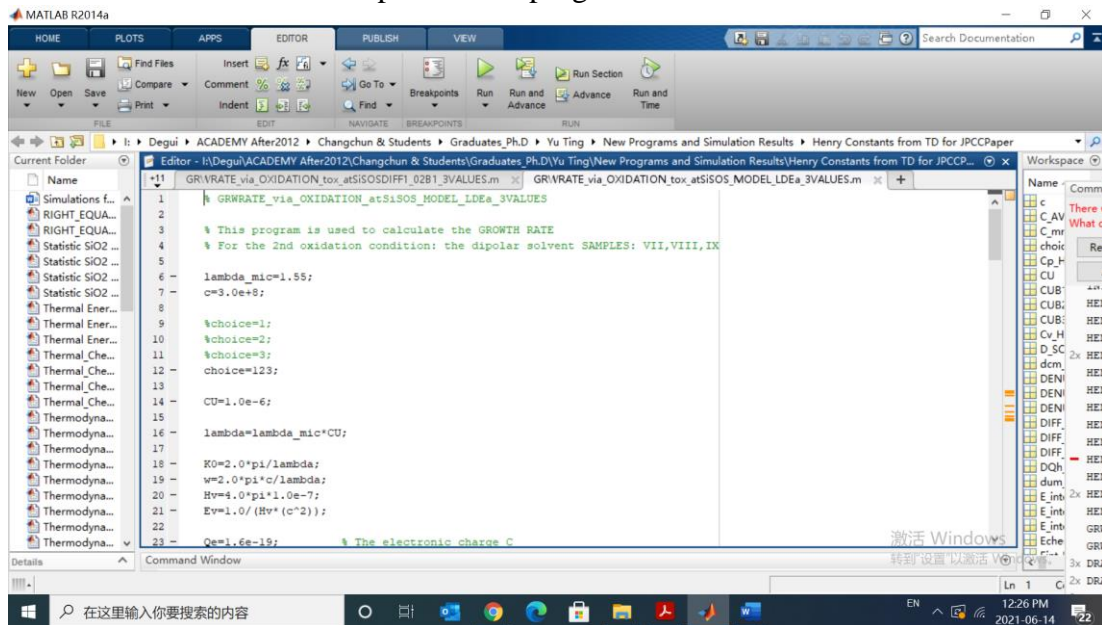
With the high initial diffusivity value of  $8.4 \times 10^{-7}$  (m<sup>2</sup>s<sup>-1</sup>), and the low initial diffusivity value  $1.0 \times 10^{-10}$  (m<sup>2</sup>s<sup>-1</sup>), for the three temperatures: 700°C, 1000°C and 1300°C, with Equation (2) and the  $E_a$  effect on the diffusivity of oxidant, we obtain the simulation results of the oxidation time dependence of SiO<sub>2</sub> growth rate with respect to four cases as shown in Figures 4(a) and 4(b), respectively. The follows are the start and end parts of the program.

```
1 GRVTH_via_OXIDATIONtox_atSISODIFFI_2B1DX.m GRVRATE_via_OXIDATIONtox_atSISOS_MODEL_2D_3TEMP.m
2 GRWRATE_via_OXIDATION_atSISOS_MODEL_2D_3TEMP
3 % This program is used to calculate the GROWTH RATE
4 % The Diffusivity effects and its Ea are also considered
5
6 lambda_mic=1.55;
7 c=3.0e+8;
8
9 %choice=1;
10 %choice=2;
11 %choice=3;
12 %choice=123;
13 %choice=456;
14 choice=123456;
15
16 CU=1.0e-6;
17
18 lambda=lambda_mic*CU;
19
20 K0=2.0*pi/lambda;
21 w=2.0*pi*c/lambda;
22 Rv=1.0*pi*1.0e-7;
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118
119
120
121
122
123
124 oxr_Si_L1=r_grw_L1/CU
125 oxr_Si_L2=r_grw_L2/CU
126 oxr_Si_L3=r_grw_L3/CU
127
128 % to plot the figure of data
129
130 if choice==123456
131 %plot(tox_hr,oxr_Si_H1,tox_hr,oxr_Si_H2,tox_hr,oxr_Si_H3,tox_hr,oxr_Si_L1,tox_hr,oxr_Si_L2,tox_hr,oxr_Si_L3)
132 semilogy(tox_hr,oxr_Si_H1,tox_hr,oxr_Si_H2,tox_hr,oxr_Si_H3,tox_hr,oxr_Si_L1,tox_hr,oxr_Si_L2,tox_hr,oxr_Si_L3)
133 xlabel('Oxidation time t_o_x (hr)')
134 ylabel('Si oxidation rate (um/min)')
135 title('Thermal oxidation rate of SiO2 in LOCOS')
136 plotedit
137 end
138
139 if choice==123
140 %plot(tox_hr,oxr_Si_H1,tox_hr,oxr_Si_H2,tox_hr,oxr_Si_H3)
141 semilogy(tox_hr,oxr_Si_H1,tox_hr,oxr_Si_H2,tox_hr,oxr_Si_H3)
142 xlabel('Oxidation time t_o_x (hr)')
143 ylabel('Si oxidation rate (um/min)')
144 title('Thermal oxidation rate of SiO2 in LOCOS')
```

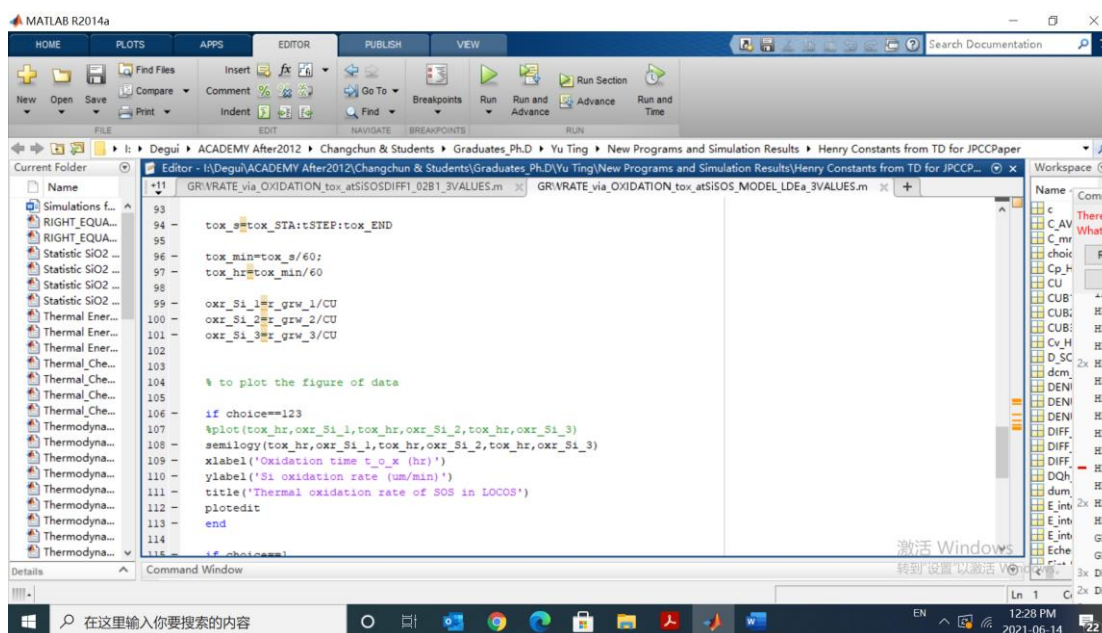
### 3. Growth rate of SiO<sub>2</sub> layer in the thermodynamic mode:

#### 3.1. Thermodynamic Model of H with Pfeffer/Ohring's model of D:

Used the following program to simulate the oxidation time dependence of SiO<sub>2</sub> growth rate at 21 temperatures in 700-1300°C, then obtain 21×21 matrix, then created the dual temp/time dependences of SiO<sub>2</sub> growth rate as shown in Figures 5(a). The follows are the start and end parts of the program.



```
1 GR\VRATE_via_OXIDATION_tox_atSISOSDIFF1_02B1_3VALUES.m
2 GR\VRATE_via_OXIDATION_tox_atSISOS_MODEL_LDEa_3VALUES.m
3
4 % This program is used to calculate the GROWTH RATE
5 % For the 2nd oxidation condition: the dipolar solvent SAMPLES: VII,VIII,IX
6
7 lambda_mic=1.55;
8
9 %choice=1;
10 %choice=2;
11 %choice=3;
12 choice=123;
13
14 CU=1.0e-6;
15
16 lambda=lambda_mic*CU;
17
18 K0=2.0*pi/lambda;
19 w=2.0*pi*c/lambda;
20 Hv=4.0*pi*1.0e-7;
21 Ev=1.0/(Hv*(c^2));
22
23 Qe=1.6e-19; % The electronic charge C
```

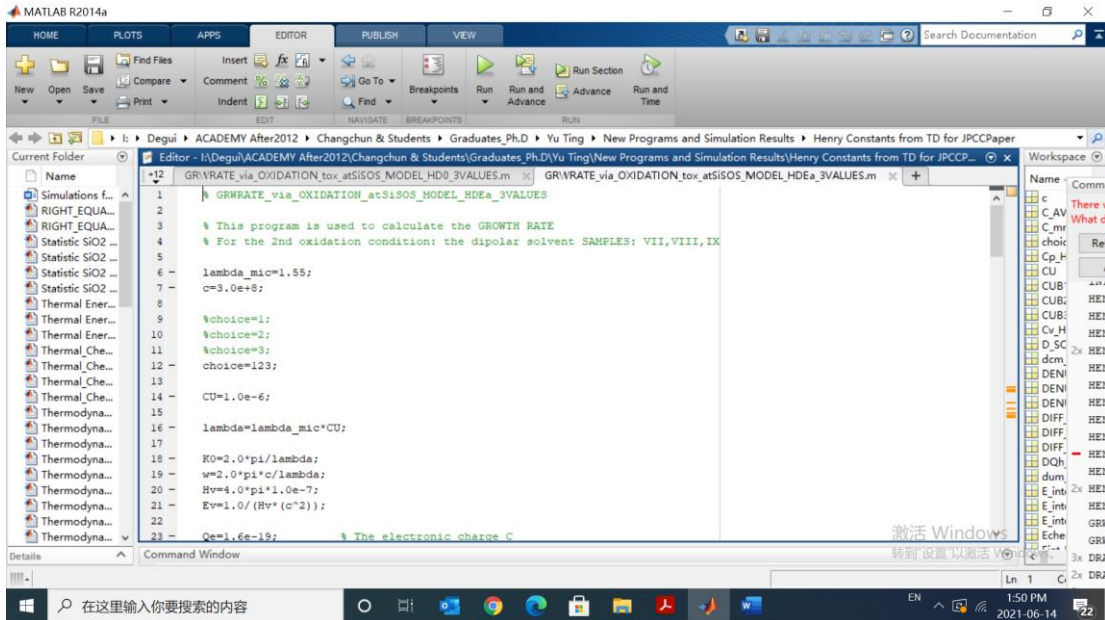


```
94 tox_s=tox_STA:cSTEP:tox_END
95
96 tox_min=tox_s/60;
97 tox_hr=tox_min/60
98
99 oxr_si_1=r_giw_1/CU
100 oxr_si_2=r_giw_2/CU
101 oxr_si_3=r_giw_3/CU
102
103
104 % to plot the figure of data
105
106 if choice==123
107 %plot(tox_hr,oxr_si_1,tox_hr,oxr_si_2,tox_hr,oxr_si_3)
108 semilogx(tox_hr,oxr_si_1,tox_hr,oxr_si_2,tox_hr,oxr_si_3)
109 xlabel('Oxidation time t_o_x (hr)')
110 ylabel('Si oxidation rate (um/min)')
111 title('Thermal oxidation rate of SOS in LOCOS')
112 plotedit
113 end
114
115 if choice==1
```

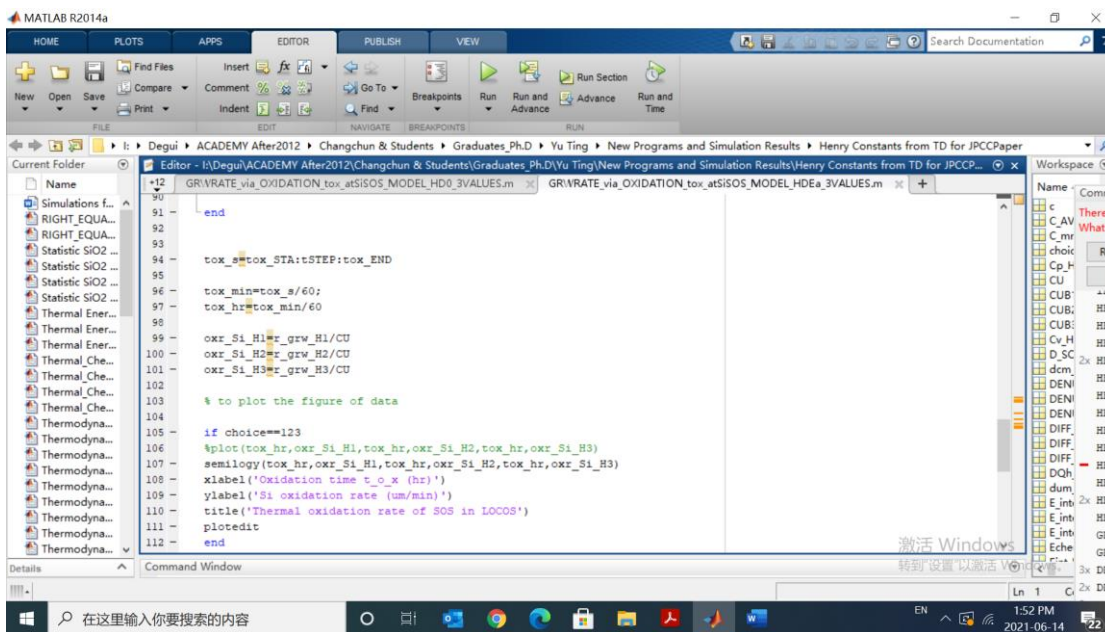


### 3.2. Thermodynamic Model of H with Kostinski's model of D:

Used the following program to simulate the oxidation time dependence of SiO<sub>2</sub> growth rate at 21 temperatures in 700-1300°C, then obtain 21×21 matrix, then created the dual temp/time dependences of SiO<sub>2</sub> growth rate as shown in Figures 5(b). The follows are the start and end parts of the program.



```
12 GR\RATE_via_OXIDATION_tox_atSiSOS_MODEL_HDEa_3VALUES.m
13 GR\RATE_via_OXIDATION_tox_atSiSOS_MODEL_HDEa_3VALUES.m
14
15 % This program is used to calculate the GROWTH RATE
16 % For the 2nd oxidation condition: the dipolar solvent SAMPLES: VII,VIII,IX
17
18 lambda_mic=1.55;
19 c=3.0e+8;
20
21 %choice=1;
22 %choice=2;
23 %choice=3;
24 choice=123;
25
26 CU=1.0e-6;
27
28 lambda=lambda_mic*CU;
29
30 R0=2.0*pi/lambda;
31 w=2.0*pi*c/lambda;
32 Hv=4.0*pi*1.0e-7;
33 Ev=1.0/(Hv*(c^2));
34
35 Qe=1.6e-19; % The electronic charge C
```

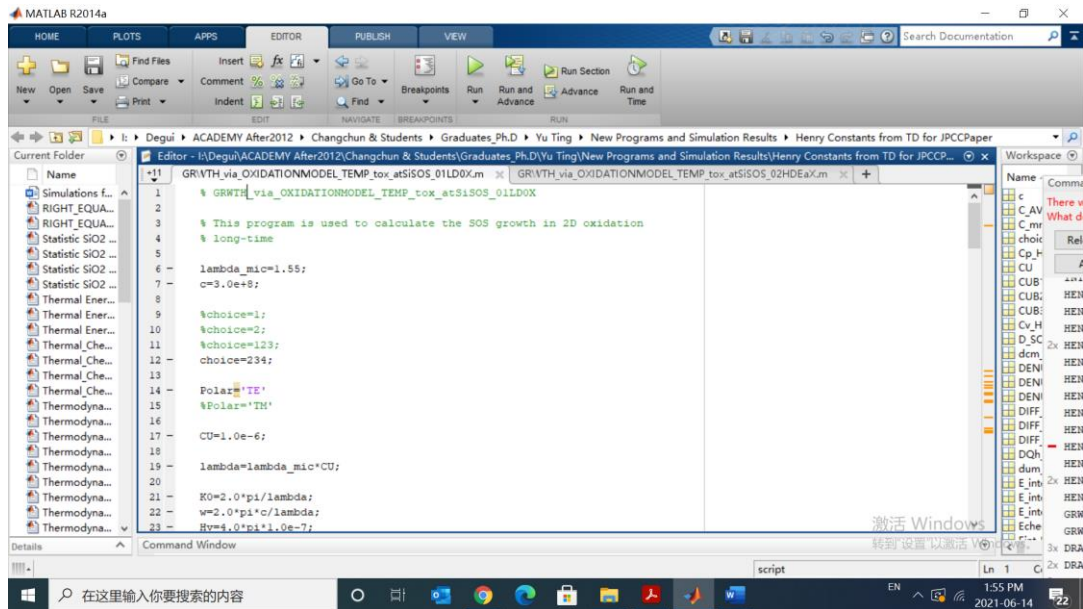


```
90
91 end
92
93
94 tox_s=tox_STA:tSTEP:tox_END
95
96 tox_min=tox_s/60;
97 tox_hr=tox_min/60
98
99 oxr_Si_H1=gr_H1/CU
100 oxr_Si_H2=gr_H2/CU
101 oxr_Si_H3=gr_H3/CU
102
103 % to plot the figure of data
104
105 if choice==123
106 %plot(tox_hr,oxr_Si_H1,tox_hr,oxr_Si_H2,tox_hr,oxr_Si_H3)
107 semilogy(tox_hr,oxr_Si_H1,tox_hr,oxr_Si_H2,tox_hr,oxr_Si_H3)
108 xlabel('Oxidation time t_o_x (hr)')
109 ylabel('Si oxidation rate (um/min)')
110 title('Thermal oxidation rate of SiO2 in LOCOS')
111 plotedit
112 end
```

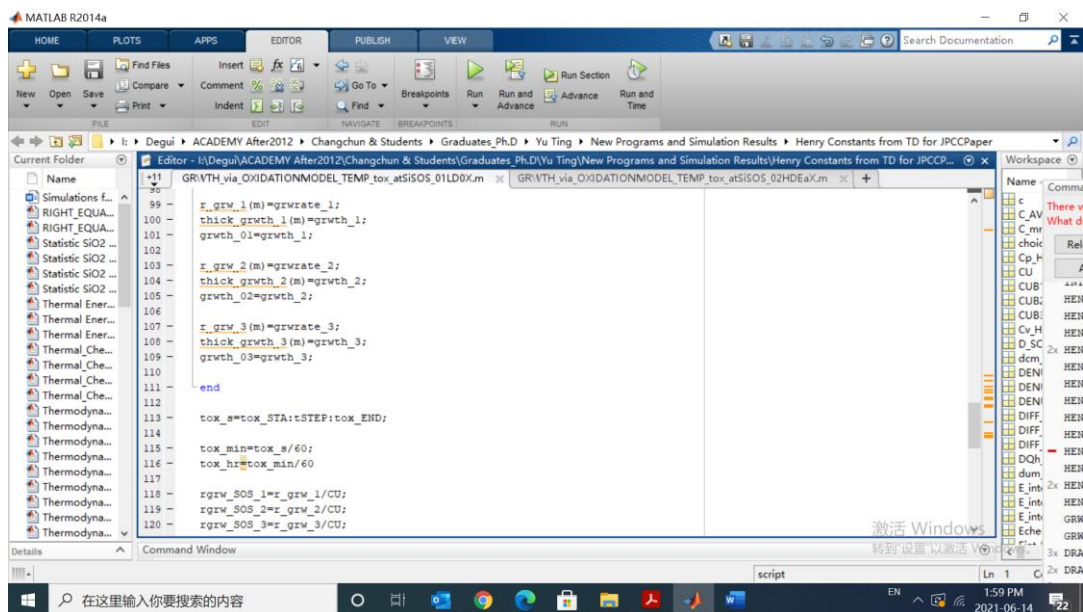
#### 4. Thickness of SiO<sub>2</sub> layer in the thermodynamic mode:

##### 4.1. Thermodynamic Model of H with Pfeffer/Ohring's model of D:

Based on simulation results for the Henry's constant and the growth rate of SiO<sub>2</sub> shown in Figures 3-5, by selecting the Pfeffer/Ohring's model of the diffusivity, with Equation (3), for the two cases in the above simulations, we obtain the simulation results of the 2-D dependences of the SiO<sub>2</sub> thickness on both the oxidation temperature and time as shown in Figures 6(a). The follows are the start and end parts of the program.



```
1 GRWTH_via_OXIDATIONMODEL_TEMP_tox_atSiSOS_01LD0X.m
2 % GRWTH_via_OXIDATIONMODEL_TEMP_tox_atSiSOS_01LD0X
3 % This program is used to calculate the SOS growth in 2D oxidation
4 % long-time
5
6 lambda_mic=1.55;
7 c=3.0e+8;
8
9 %choice=1;
10 %choice=2;
11 %choice=123;
12 choice=234;
13
14 Polar='TE';
15 %Polar='TM';
16
17 CU=1.0e-6;
18
19 lambda=lambda_mic*CU;
20
21 KO=2.0*pi/lambda;
22 w=2.0*pi*c/lambda;
23 Hv=1.0*pi*1.0e-7;
```



```
99
100 r_grw_1(m)=grwrate_1;
101 thick_grwth_1(m)=grwth_1;
102 grwth_01=grwth_1;
103
104 r_grw_2(m)=grwrate_2;
105 thick_grwth_2(m)=grwth_2;
106 grwth_02=grwth_2;
107
108 r_grw_3(m)=grwrate_3;
109 thick_grwth_3(m)=grwth_3;
110 grwth_03=grwth_3;
111 end
112
113 tox_s=tox_STA:tSTEP:tox_END;
114
115 tox_min=tox_s/60;
116 tox_hr=tox_min/60;
117
118 rgrw_SOS_1=r_grw_1/CU;
119 rgrw_SOS_2=r_grw_2/CU;
120 rgrw_SOS_3=r_grw_3/CU;
```

## 4.2. Thermodynamic Model of H with Kostinski's model of D:

Based on simulation results for the Henry's constant and the growth rate of  $\text{SiO}_2$  shown in Figures 3-5, by selecting the Kostinski's model of the diffusivity, with Equation (3), for the two cases in the above simulations, we obtain the simulation results of the 2-D dependences of the  $\text{SiO}_2$  thickness on both the oxidation temperature and time as shown in Figures 6(b). The follows are the start and end parts of the program.

```
1 % GRWTH_via_OXIDATIONMODEL_TEMP_tox_atSiSOS_02HDEaX
2
3 % This program is used to calculate the SOS growth in 2D oxidation
4 % long-time
5
6 lambda_mic=1.55;
7 c=3.0e+9;
8
9 %choice=1;
10 %choice=2;
11 %choice=123;
12 choice=234;
13
14 %Polar='TE'
15 %Polar='TM'
16
17 CU=1.0e-6;
18
19 lambda=lambda_mic*CU;
20
21 K0=2.0*pi/lambda;
22 w=2.0*pi*c/lambda;
23 Hv=1.0*pi*1.0e-7;
```

```
103 r_gw_1(m)=grwrate_1;
104 thick_gwth_1(m)=grwth_1;
105 grwth_01=grwth_1;
106
107 r_gw_2(m)=grwrate_2;
108 thick_gwth_2(m)=grwth_2;
109 grwth_02=grwth_2;
110
111 r_gw_3(m)=grwrate_3;
112 thick_gwth_3(m)=grwth_3;
113 grwth_03=grwth_3;
114
115 end
116
117 tox_s=tox_STA:tSTEP:tox_END;
118
119 tox_min=tox_s/60;
120 tox_hr=tox_min/60
121
122 rgrw_SOS_1=r_gw_1/CU;
123 rgrw_SOS_2=r_gw_2/CU;
124 rgrw_SOS_3=r_gw_3/CU;
```



## 5. Henry's law constant in the empirical model:

5.1. Empirical Model of H with the molecule interaction parameters:  $\sigma_{ab}^* = 1.0$ ,  $\varepsilon_{ab}^*$

has three values as 0.7071, 0.9747 and 1.2247

For Henry's law constant from the empirical model extracted from the published data, with Equation (7), the simulation results of Henry's constant dependences on temperature with respect to the above three values of  $\varepsilon_{ab}^*$  and three values of  $\sigma_{ab}^*$  as shown in Figure 7(a). The follows are the start and end parts of the program.

```
10 GRVRATE_via_OXIDATION_box_atSISODIFF1_02A1_3VALUES.m HENRYCNST_via_CHEMPOTENTIAL_atSISOS_01A_SINGLE.m
11 HENRYCNST_via_CHEMPOTENTIAL_atSISOS_01A_SINGLE
12 % This program is used to calculate the Henry's law constant in OXIDATION
13 % Of difference of O1a from O1 is that the energy parameter is introduced
14 % for the nonpolar solvent (moull1_star)^2=0 Systems: I, II and III
15 lambda_mic=1.55;
16 c=3.0e+8;
17 choice=1;
18 %choice=2;
19 CU=1.0e-6;
20 lambda=lambda_mic*CU;
21 K0=2.0*pi/lambda;
22 w=2.0*pi*c/lambda;
23 Hv=4.0*pi*1.0e-7;
24 Ev=1.0/(Hv*(c^2));
25 Qe=1.6e-19; % The electronic charge C
26 k_biz=1.38e-23; % Boltzman constant
27
28
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34
35
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94
95
96 T1_star=TK/epcab1_KB;
97 T2_star=TK/epcab2_KB;
98 T3_star=TK/epcab3_KB;
99
100 H_O2_1=(role_O2mlc*k_biz*TK)*exp(-0.5/epcab1_KB);
101 H_O2_2=(role_O2mlc*k_biz*TK)*exp(-8.0/epcab2_KB+T2_star*5.0/TK);
102 H_O2_3=(role_O2mlc*k_biz*TK)*exp(-14.7/epcab3_KB+T3_star*9.0/TK);
103
104 % To set the loop of SiO2 growth rate
105
106 H2O_1(m)=H2_O_1;
107 H2O_2(m)=H2_O_2;
108 H2O_3(m)=H2_O_3;
109
110 end
111
112 T_deg=TEMP_STA:TSTEP:TEMP_END
113
114 HENRY_CNT1=H2O_1;
115 HENRY_CNT2=H2O_2;
116 HENRY_CNT3=H2O_3;
117
118 if choice==1
```



## 5.2 Empirical Model of H with the molecule interaction parameters: parameter

$$\varepsilon_{ab}^* = 1.0, \quad \sigma_{ab}^* \text{ has three values as } 0.750, 0.975 \text{ and } 0.625$$

For Henry's law constant from the empirical model extracted from the published data, with Equation (7), the simulation results of Henry's constant dependences on temperature at  $\varepsilon_{ab}^*=1.0$  and the three values of  $\sigma_{ab}^*$  as shown in Figure 7(b). The follows are the start and end parts of the program.

```

1 GR\VRATE_via_OXIDATIONtox_atSISODIFFI_02A1_3VALUES.m HENRYCNST_via_CHEMPOTENTIAL_atSISOS_01B_SINGLE.m
2 HENRYCNST_via_CHEMPOTENTIAL_atSISOS_01B_SINGLE
3
4 % This program is used to calculate the Henry's law constant in OXIDATION
5 % Of difference of 01B from 01A is that the size parameter is introduced
6 % for the nonpolar solvent (moull1_star)^2=0 Systems: IV, V and VI
7
8 lambda_mic=1.55;
9 c=3.0e+8;
10
11 %choice=1;
12 choice=2;
13
14 Polar='TE';
15 %Polar='TH';
16
17 CD=1.0e-6;
18
19 lambda=lambda_mic*CU;
20
21 K0=2.0*pi/lambda;
22 w=2.0*pi*c/lambda;
23 Hv=4.0*pi*1.0e-7;
24 Ev=1.0/(Hv*(c^2));
25
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92
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96
97
98
99
100
101 T1_star=TK/epcab1_KB;
102 T2_star=TK/epcab2_KB;
103 T3_star=TK/epcab3_KB;
104
105 H_O2_1=(role_O2mlc*k_b1z*TK)*exp(-5.2/epcab1_KB+T1_star*3.5/TK);
106 H_O2_2=(role_O2mlc*k_b1z*TK)*exp(-6.9/epcab2_KB+T2_star*4.5/TK);
107 H_O2_3=(role_O2mlc*k_b1z*TK)*exp(-7.8/epcab3_KB+T3_star*4.5/TK);
108
109 % To set the loop of SiO2 growth rate
110
111 HO2_1(m)=H_O2_1;
112 HO2_2(m)=H_O2_2;
113 HO2_3(m)=H_O2_3;
114
115 end
116
117 T_deg=TEMP_STA:TSTEP:TEMP_END;
118
119 HENRY_CNT1=HO2_1
120 HENRY_CNT2=HO2_2;
121 HENRY_CNT3=HO2_3;
122

```

6. Growth rate of silicon dioxide (SiO<sub>2</sub>) in the empirical mode:

6.1. Growth rate of SiO<sub>2</sub> with the molecule interaction parameters:

$$\sigma_{ab}^* = 1.0, \quad \varepsilon_{ab}^* = 0.7071$$

For System VII, by selecting the Pfeiffer/Ohring's model for the diffusivity of H<sub>2</sub>O in SiO<sub>2</sub> as  $D_0 = 1.0 \times 10^{-10}$  (m<sup>2</sup>s<sup>-1</sup>)/ $E_a = 0$ , with Equation (2), we simulate the thermal oxidation rates depending on both the oxidation temperature and time for these two systems as shown in Figures 8(a). The follows are the start and end parts of the program.

```

1 GRWRATE_via_OXIDATIONtox_atSISOS_MODEL_HDEa_3VALUES.m GRWRATE_via_OXIDATIONtox_atSISOSDIFF1_02A1_3VALUES.m
2 % GRWRATE_via_OXIDATIONtox_atSISOSDIFF1_02A1_3VALUES
3
4 % This program is used to calculate the GROWTH RATE
5 % For the 2nd oxidation condition: the dipolar solvent SAMPLES: VII,VIII,IX
6
7 lambda_mic=1.55;
8 c=3.0e+8;
9
10 %choice=1;
11 %choice=2;
12 %choice=3;
13 choice=123;
14
15 CU=1.0e-6;
16
17 lambda=lambda_mic*CU;
18
19 K0=2.0*pi/lambda;
20 w=2.0*pi*c/lambda;
21 Hv=4.0*pi*1.0e-7;
22 Ev=1.0/(Hv*(c^2));
23
24 Qe=1.6e-19; % The electronic charge C

```

```

74
75 NUMER_r_3=H_02_3*P_g*ks;
76 DENUM_r_3=(r01e_02/2)*(1+ks/h_3+ks*tox_s/D_50);
77
78 % To set the loop of SiO2 growth rate
79
80 r_giw_1(m)=NUMER_r_1/DENUM_r_1;
81 r_giw_2(m)=NUMER_r_2/DENUM_r_2;
82 r_giw_3(m)=NUMER_r_3/DENUM_r_3;
83
84 end
85
86
87 tox_s=tox_STA:tSTEP:tox_END
88
89 tox_min=tox_s/60;
90 tox_hr=tox_min/60
91
92 oxr_Si_1=r_giw_1/CU
93 oxr_Si_2=r_giw_2/CU
94 oxr_Si_3=r_giw_3/CU
95
96 % to plot the figure of data

```

## 6.2 Growth rate of SiO<sub>2</sub> with the molecule interaction parameters:

$$\varepsilon_{ab}^* = 1.0, \quad \sigma_{ab}^* = 0.625$$

For System XII, by selecting the Pfeffer/Ohring's model for the diffusivity of H<sub>2</sub>O in SiO<sub>2</sub> as  $D_0 = 1.0 \times 10^{-10} \text{ (m}^2\text{s}^{-1})/E_a = 0$ , with Equation (2), we simulate the thermal oxidation rates depending on both the oxidation temperature and time for these two systems as shown in Figures 8(b). The follows are the start and end parts of the program.

```

1  % GRRATE_via_OXIDATION_atSiSOSDIFFI_02A1_3VALUES
2
3  % This program is used to calculate the GROWTH RATE
4  % For the 2nd oxidation condition: the dipolar solvent SAMPLES: VII,VIII,IX
5
6  lambdaMic=1.55;
7  c=3.0e+8;
8
9  %choice=1;
10 %choice=2;
11 %choice=3;
12 choice=123;
13
14 CU=1.0e-6;
15
16 lambda=lambdaMic*CU;
17
18 K0=2.0*pi/lambda;
19 w=2.0*pi*c/lambda;
20 Hv=4.0*pi*1.0e-7;
21 Ev=1.0/(Hv*(c^2));
22
23 Qe=1.6e-19; % The electronic charge C
    
```

```

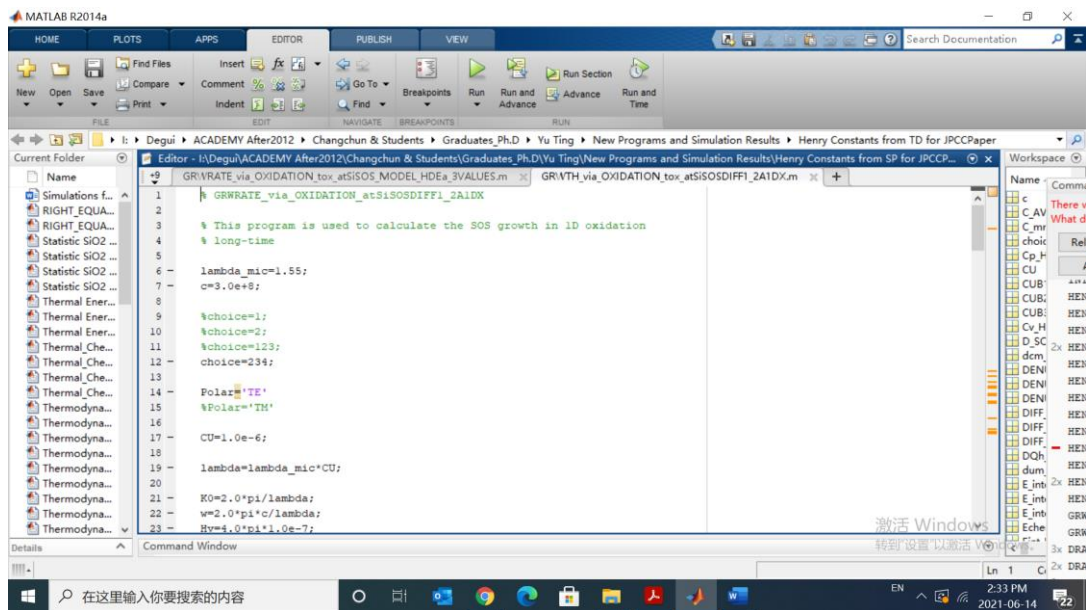
73 GRRATE_via_OXIDATION_tox_atSiSOS_MODEL_HDEa_3VALUES.m
74 DENUM_r_2=(r01e_02/2)*(1+ks/h_2+ks*tox_s/D_S0);
75 NUMER_r_3=H_02_3*p_g*ks;
76 DENUM_r_3=(r01e_02/2)*(1+ks/h_3+ks*tox_s/D_S0);
77
78 % To set the loop of SiO2 growth rate
79
80 r_gw_1(m)=NUMER_r_1/DENUM_r_1;
81 r_gw_2(m)=NUMER_r_2/DENUM_r_2;
82 r_gw_3(m)=NUMER_r_3/DENUM_r_3;
83
84 end
85
86 tox_s=tox_STA:tSTEP:tox_END
87
88
89 tox_min=tox_s/60;
90 tox_hr=tox_min/60
91
92 oxr_Si_1=r_gw_1/CU
93 oxr_Si_2=r_gw_2/CU
94 oxr_Si_3=r_gw_3/CU
    
```



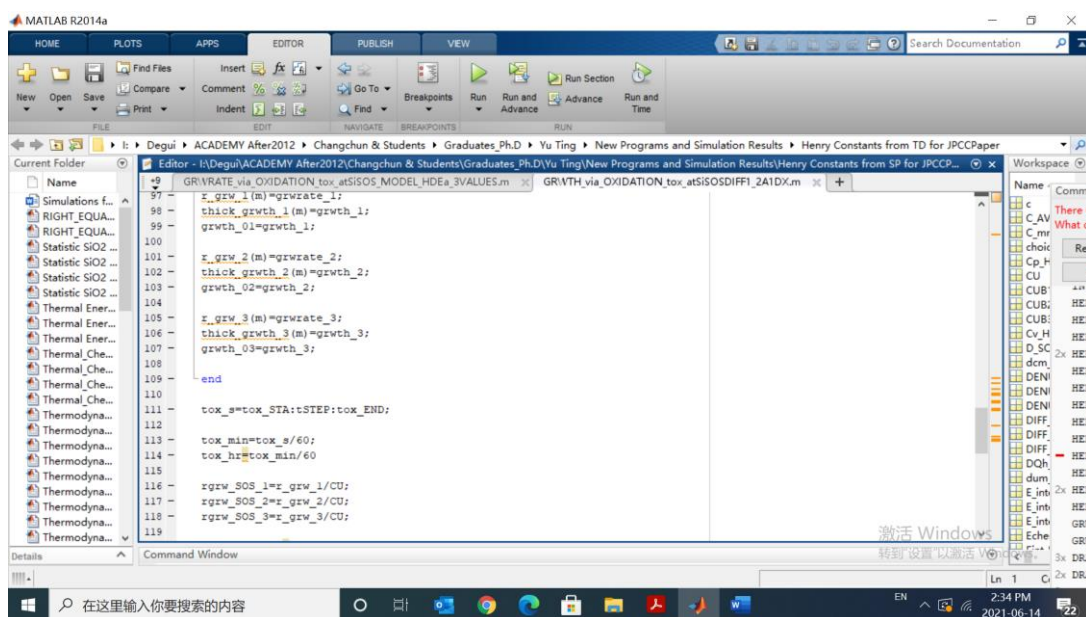
## 7. Thickness of SiO<sub>2</sub> layer in the empirical mode:

### 7.1. Molecule interaction parameters: $\sigma_{ab}^* = 1.0$ , $\varepsilon_{ab}^* = 0.7071$

For System VII, by selecting the Pfeiffer/Ohring's model for the diffusivity of H<sub>2</sub>O in SiO<sub>2</sub> as  $D_0 = 1.0 \times 10^{-10}$  (m<sup>2</sup>s<sup>-1</sup>)/ $E_a = 0$ , with Equation (3) and the same values of parameters as used in the above simulations of silicon oxidation rates, we obtain the simulation results of the 2-D dependences of SiO<sub>2</sub> thickness of System: VII as shown in Figure 9(a). The follows are the start and end parts of the program.



```
1  GRVVRATE_via_OXIDATION_tox_atSiSOS_MODEL_HDEa_3VALUES.m
2  GRVVRATE_via_OXIDATION_tox_atSiSOSDIFF1_2AIDX
3  % This program is used to calculate the SOS growth in 1D oxidation
4  % long-time
5
6  lambda_mic=1.55;
7  c=3.0e+8;
8
9  %choice=1;
10 %choice=2;
11 %choice=123;
12 choice=234;
13
14 Polar='TE';
15 %Polar='TH';
16
17 CU=1.0e-6;
18
19 lambda=lambda_mic*CU;
20
21 K0=2.0*pi/lambda;
22 w=2.0*pi*c/lambda;
23 Hv=4.0*pi*1.0e-7;
```



```
97  r_grw_1(m)=grwrate_1;
98  thick_grwth_1(m)=grwth_1;
99  grwth_01=grwth_1;
100
101  r_grw_2(m)=grwrate_2;
102  thick_grwth_2(m)=grwth_2;
103  grwth_02=grwth_2;
104
105  r_grw_3(m)=grwrate_3;
106  thick_grwth_3(m)=grwth_3;
107  grwth_03=grwth_3;
108
109  end
110
111  tox_s=tox_STA:tSTEP:tox_END;
112
113  tox_min=tox_s/60;
114  tox_hr=tox_min/60;
115
116  rgrw_SOS_1=r_grw_1/CU;
117  rgrw_SOS_2=r_grw_2/CU;
118  rgrw_SOS_3=r_grw_3/CU;
119
```

7.2 Molecule interaction parameters:  $\varepsilon_{ab}^* = 1.0$ ,  $\sigma_{ab}^* = 0.625$

For System XII, by selecting the Pfeffer/Ohring's model for the diffusivity of  $H_2O$  in  $SiO_2$  as  $D_0 = 1.0 \times 10^{-10} \text{ (m}^2\text{s}^{-1}\text{)}/E_a = 0$ , with Equation (3) and the same values of parameters as used in the above simulations of silicon oxidation rates, we obtain the simulation results of the 2-D dependences of  $SiO_2$  thickness of System: XII as shown in Figure 9(b). The follows are the start and end parts of the program.

