



RD-50 Vilnius 4.05 – 6.05.2007

Kinetic studies for n-irradiated Si with enhanced carbon concentration

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OUTLINE

- **Motivation**
- **Experimental details:**
 - measurement technique,**
 - sample preparation,**
 - annealing processes**
- **Experimental results**
- **Approximation of the experimental data by a first order diffusion limited model**
- **Fitting procedure by a multi-reaction model**
- **Results of fitting procedures**
- **Summary**



Motivation

To find out how the carbon concentration affects the kinetics of annihilation and generation of the main oxygen related complexes VO and VO₂ in neutron irradiated silicon



Experimental details

Sample preparation:

- **Silicon 2 mm thick wafers were cut from n and p type CZ-Si and n type FZ-Si crystals with different carbon concentration.**
- **Oxygen concentration for CZ-Si crystals was $9.5-12 \cdot 10^{17} \text{at/cm}^2$**
- **Calculation of O and C concentrations from FTIR absorption measurements individually for each wafer before irradiation with taking into account its radial distribution.**
- **Irradiation with the neutron dose of $1 \cdot 10^{17} \text{n/cm}^2$**
- **Cutting the wafers into samples of dimension $8 \times 12 \times 2 \text{mm}^3$**
- **Calculation O and C concentrations individually for each sample after irradiation**



Heat treatment

- Isothermal annealings at 300°C, 312°C, 325°C, 330°C and 350°C for 5- 2000 minutes were performed
- After each annealing process the absorption measurements were carried out and concentrations of oxygen and carbon were determined from the intensity of absorption lines at 1107cm⁻¹ and 607cm⁻¹, respectively.



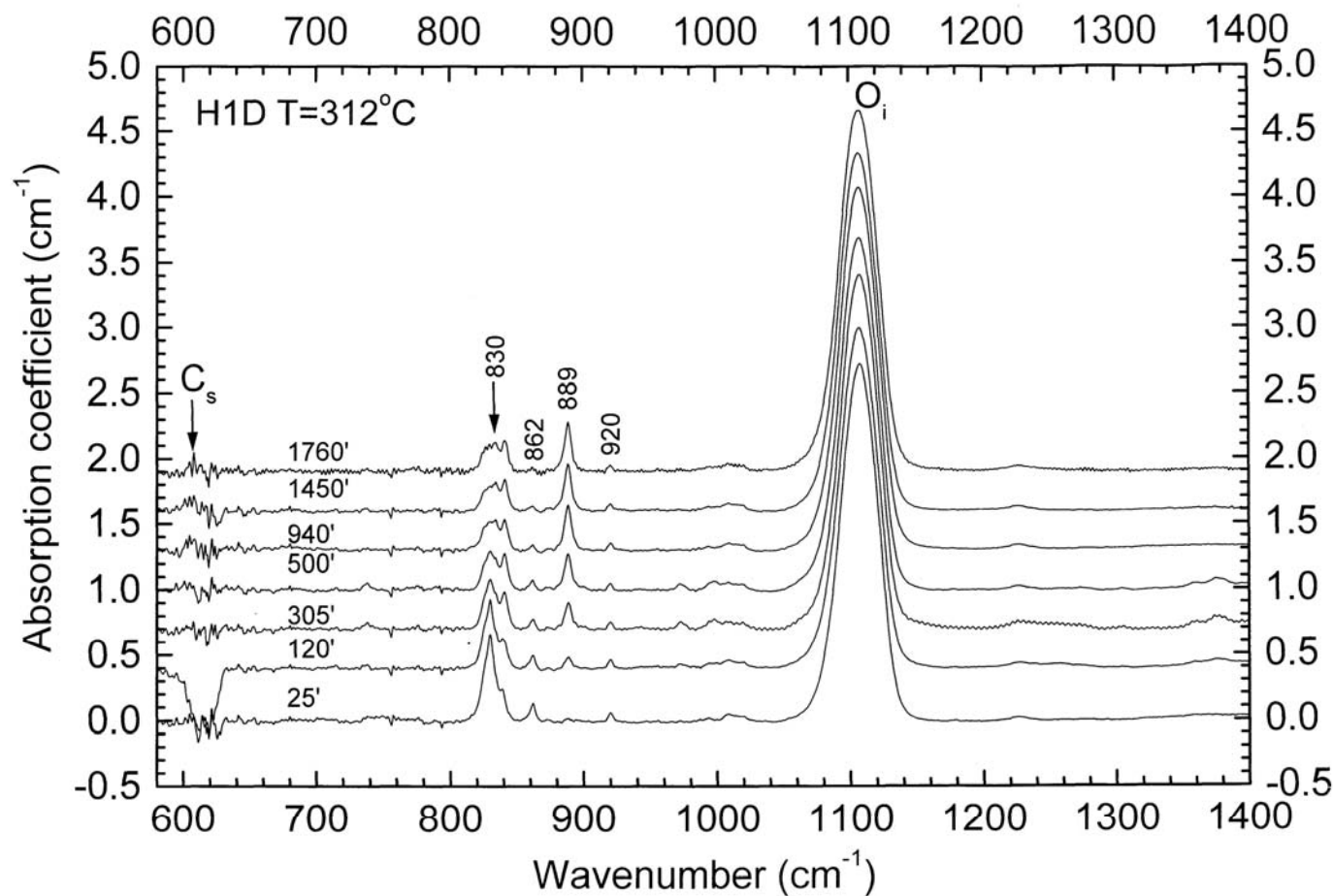
Basic characteristics of as-grown and as-irradiated wafers

TABLE I Parameters for studied crystals

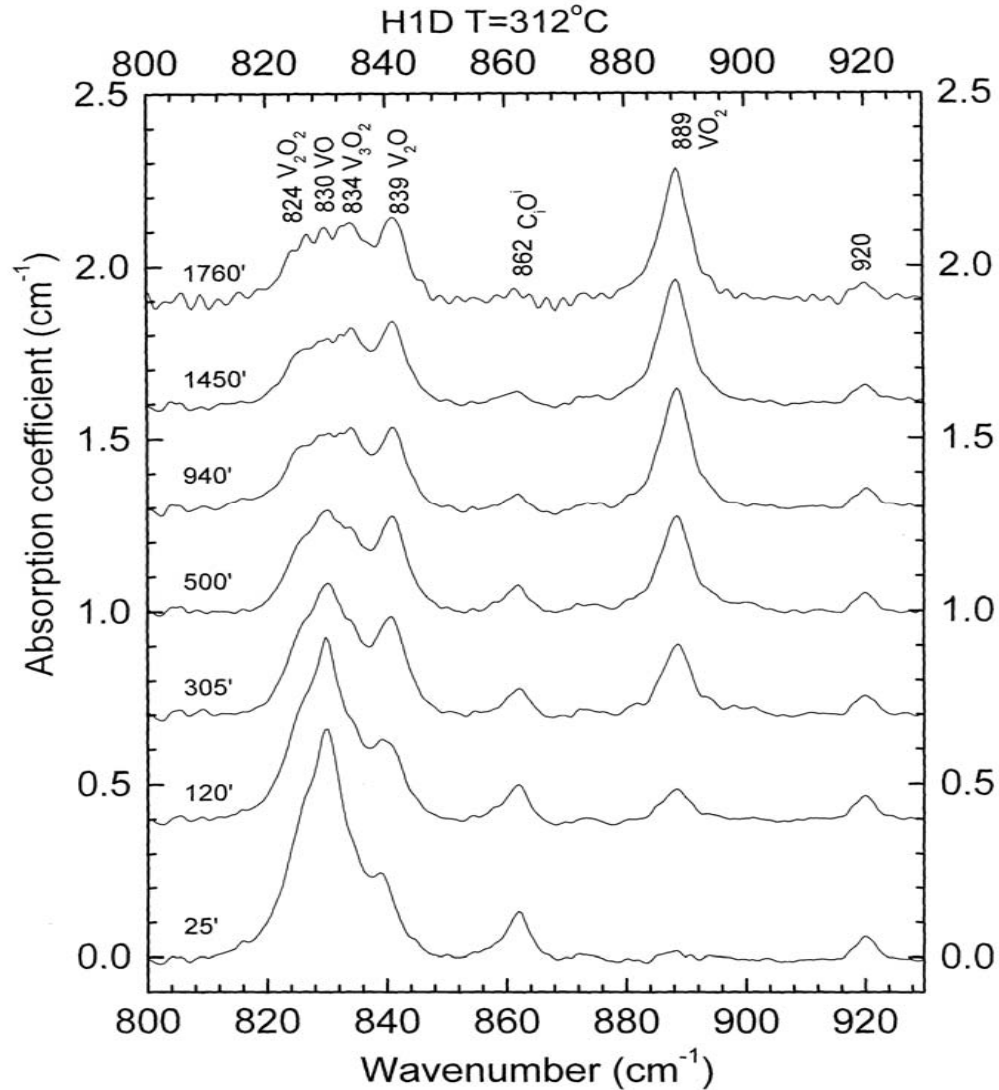
Dose	crystal	type	resistivity omcm	[O]*10 ¹⁷ center	[O]*10 ¹⁷ edge	[C]*10 ¹⁶	abs.coeff. VO 831cm ⁻¹ center	abs. coeff. VO 831cm ⁻¹ edge	abs. coeff. C ₁ -O 861 cm ⁻¹	D[O] *10 ¹⁷ at/cm ⁻³ center	D[O] *10 ¹⁷ at/cm ⁻³ edge	D[C] cent/edge *10 ¹⁶ at/cm ⁻³
neutron irradiated 1*10 ¹⁷ n/cm ²	HL1			8.77	6.24	1.7-<det	0.576	0.471	0.096-0.086	0.63	1.2	3.3/4.4
	HL2			9.88	8.5	0.58-1.1	0.555	0.515	0.13-0.099	0.36	0.9	3.7/3.3
	HL3			8.7	8.01	-	0.53	0.495	0.035-0.045	1.4	1.2	2.7
	HL4			9.02	8.7	1.09-<det	0.54	0.52	0.07/0.08	0.56	0.9	2/2.4
	HL5			11	10.6	-	0.508	0.517	-	1.3	2.4	<det
	HL6			1.69	1.69	<det	0.253	0.253	0.0219	0.15	0.15	<det
	HL7			-	-	2.18	-	-	-	-	-	2.6
nonirradiated	L1	n	14	9.4	7.5	5.0-4.9-4.4	-		-			
	L2	p	16	10.24	9.4	4.3	-		-			
	L3	p	8	10.09	9.1	2.75-2.6	-		-			
	L4	p	8	9.58	8.97	3.03/2.4	-		-			
	L5	p	10	12.6	12.4	0.8	-		-			
	L6	n	800	1.84	1.83	1	-		-			
	L7	p	800	-	-	4.85	-		-			



Absorption spectra for sample from H1 crystal versus time of annealing at $T=312^{\circ}\text{C}$ $[\text{C}]=5 \cdot 10^{16}$ at/cm³ $[\text{O}]=9.4 \cdot 10^{17}$ at/cm³



VO - 830cm-1
C_iO_i - 862cm-1
VO₂ - 889cm-1
O_i - 1107cm-1
C_s - 607cm-1

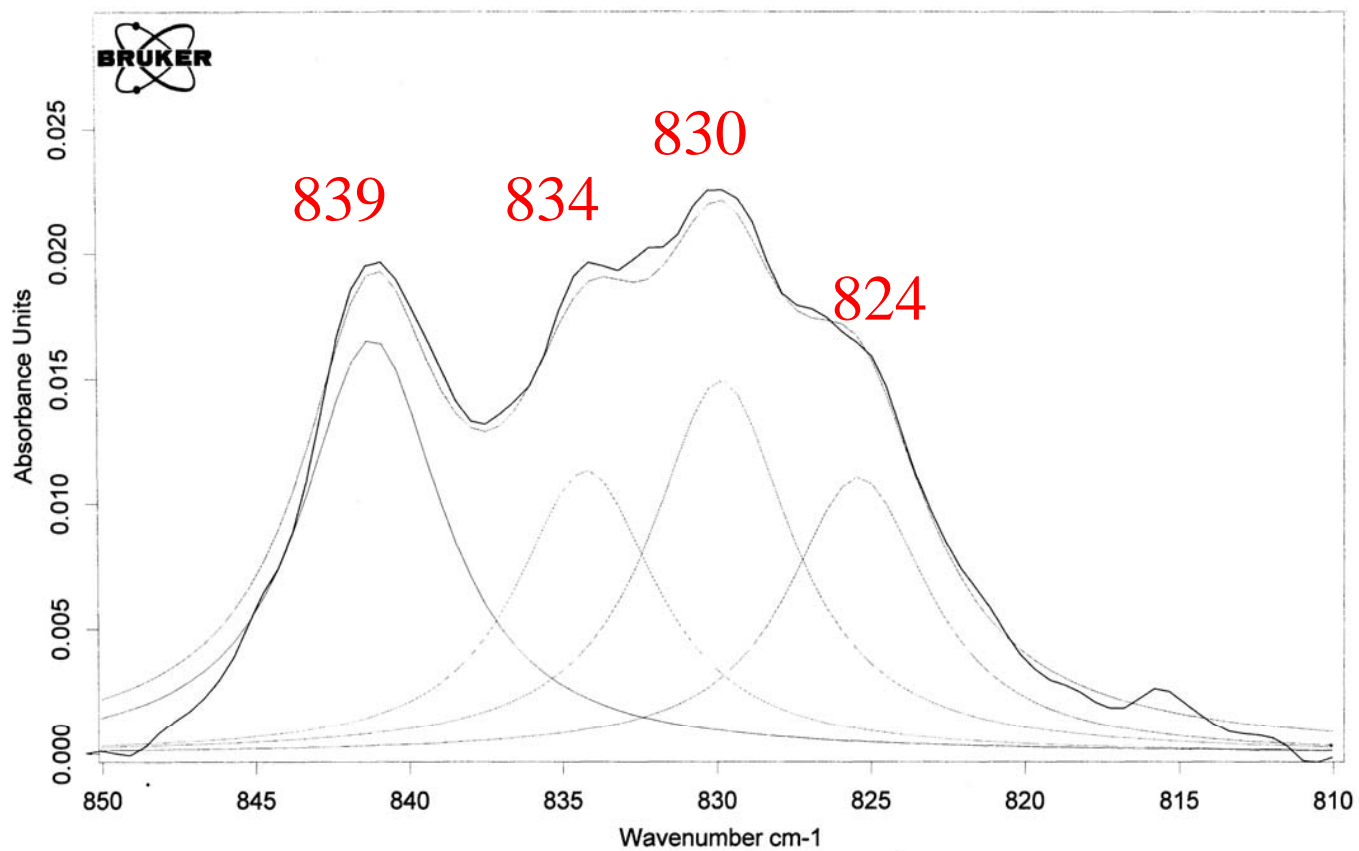


Absorption spectra for oxygen-related defects

- VO - 830cm^{-1}
- C_iO_i - 862cm^{-1}
- VO_2 - 889cm^{-1}
- V_2O - 839cm^{-1}
- V_2O_2 - 824cm^{-1}
- V_3O_2 - 834cm^{-1}



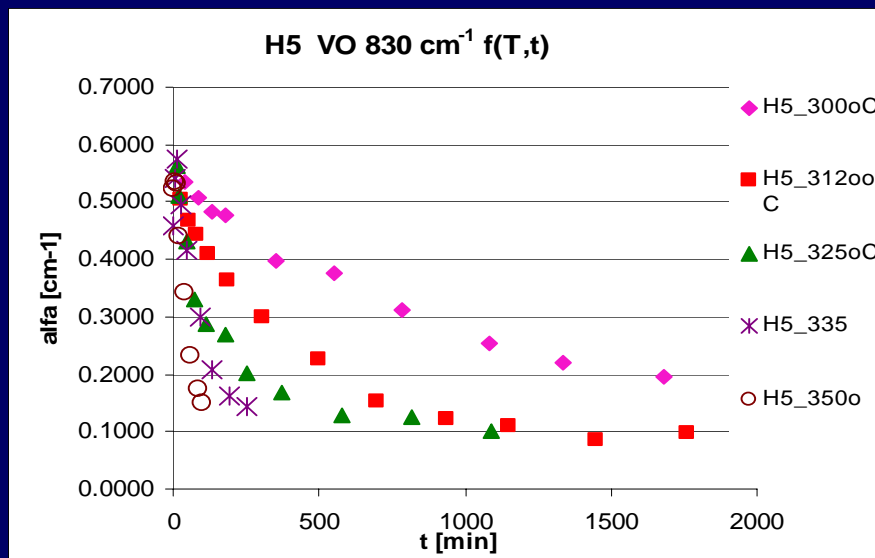
Deconvolution



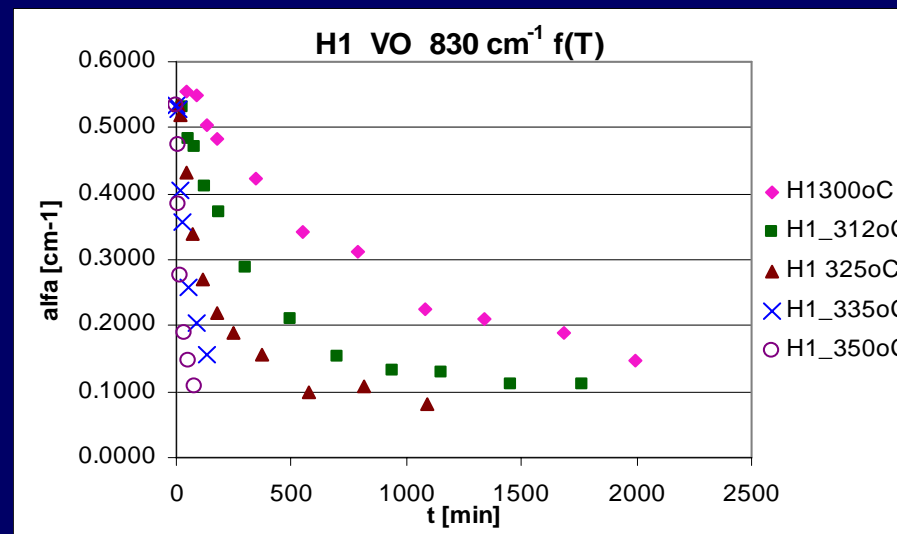
D:\ROMA\Si\Si_ irradiated\ir-irr_2004\DELTA\wvorzewane\zb_f(czasu)\FIT\T300\H1K\H1K_TX10\BL_H1K_TX10.0	Si-irr_1*10^17n/cm2_TX10=3	2005/03/09
D:\opus\WORK\FIT_1793		18/11/2005
D:\opus\WORK\FIT_1794		18/11/2005
D:\opus\WORK\FIT_1795		18/11/2005
D:\opus\WORK\FIT_1796		18/11/2005
D:\opus\WORK\FIT_1797		18/11/2005



The intensity of the absorption band at 830 cm⁻¹ related to VO defects versus time of annealing



[C]=0.8*10¹⁶ at/cm³



[C]=5*10¹⁶ at/cm³



Model of diffusion limited processes (1)

The rate equation for defect N which disappears through a first-order diffusion-limited processes $X+N \rightleftharpoons Z$

$$-\frac{\partial[N]}{\partial t} = k * [X]_{t=0} * [N]$$

$$k = 4\pi RD$$

$$D = D_X + D_N$$

R – rate capture radius;
 D - diffusion coefficient ;
 k -rate constant ;



Model of diffusion limited processes (2)

$$[N] = [N]_{t=0} * \exp(-k t)$$

$$k * t = \ln \frac{[N]}{[N]_{t=0}}$$

$$k = k_0 * \exp\left(-\frac{E_a}{k_B T}\right)$$

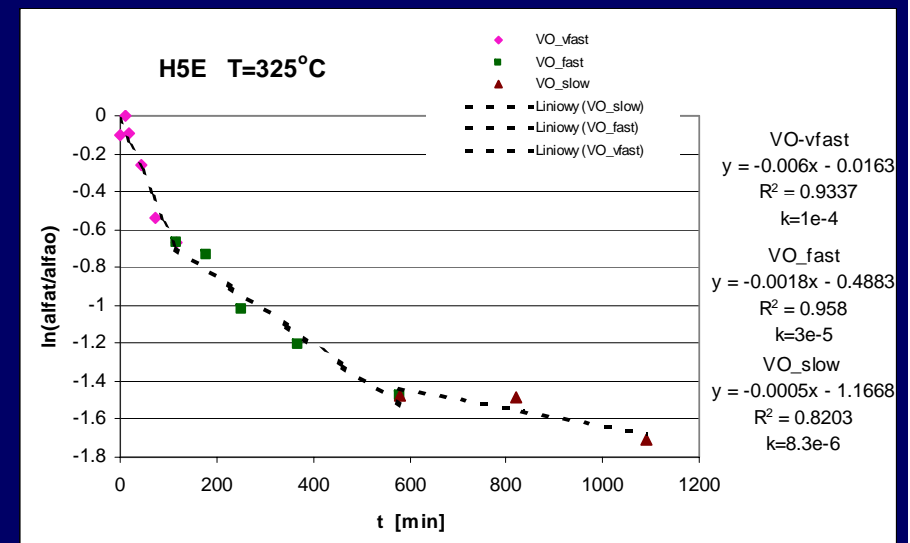
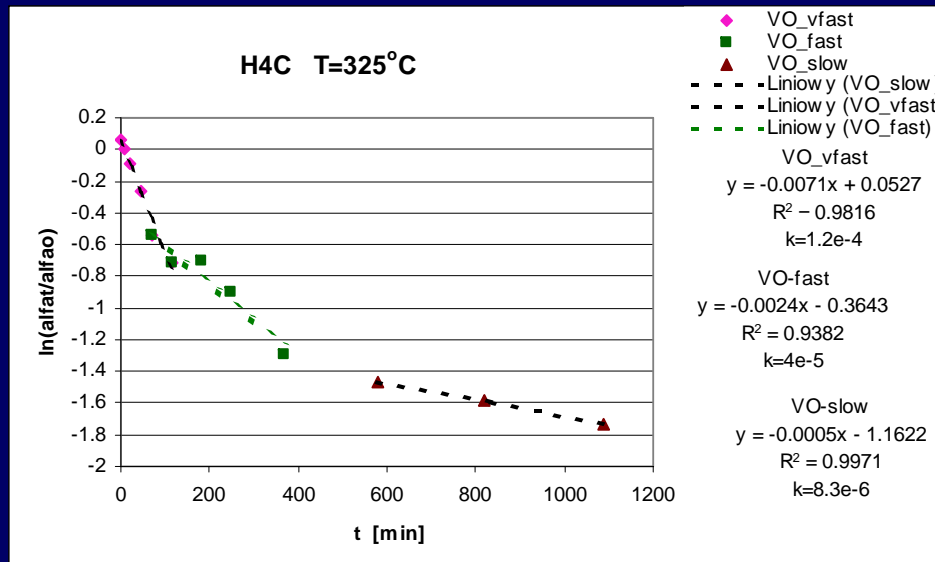
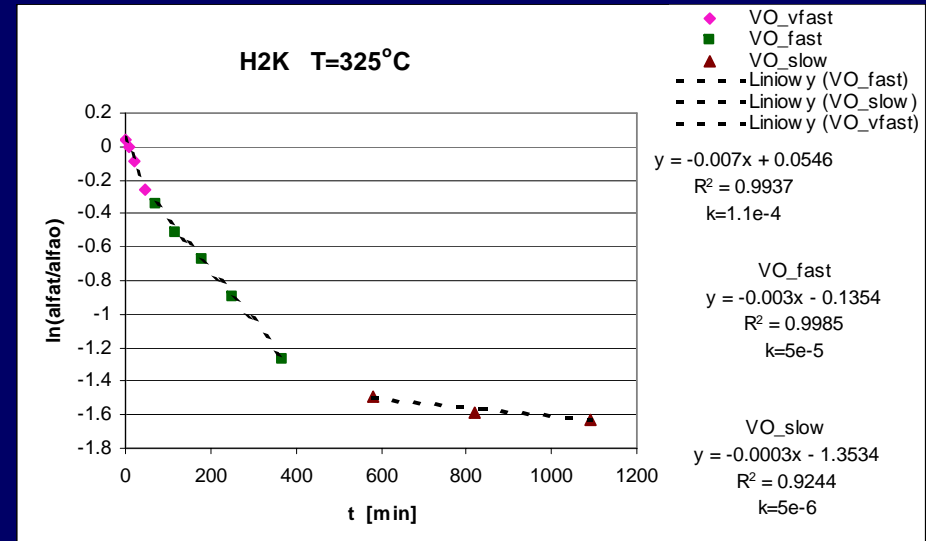
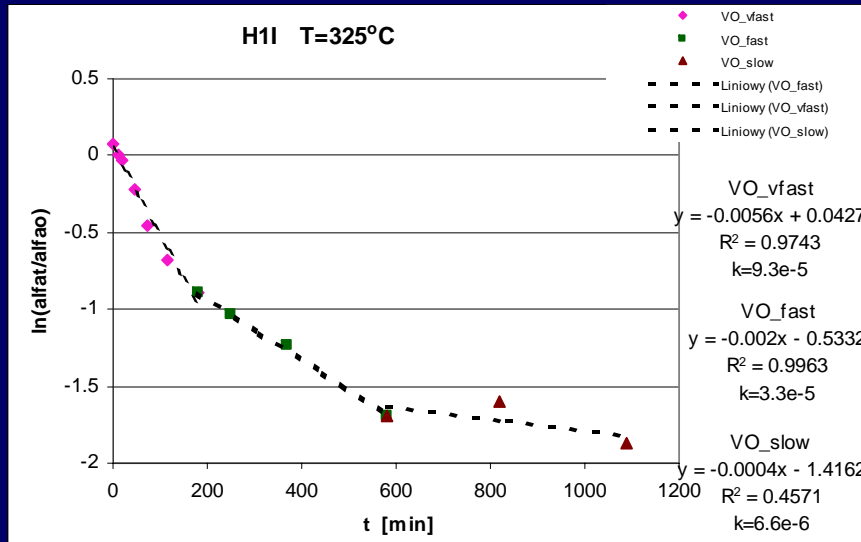
E_a – activation energy for the process

From the temperature dependence of the reaction rate k the activation energy is determined



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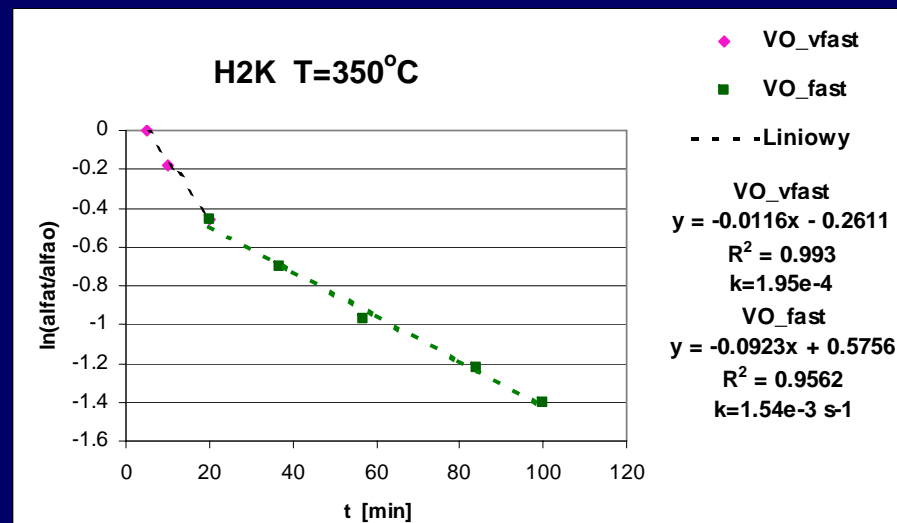
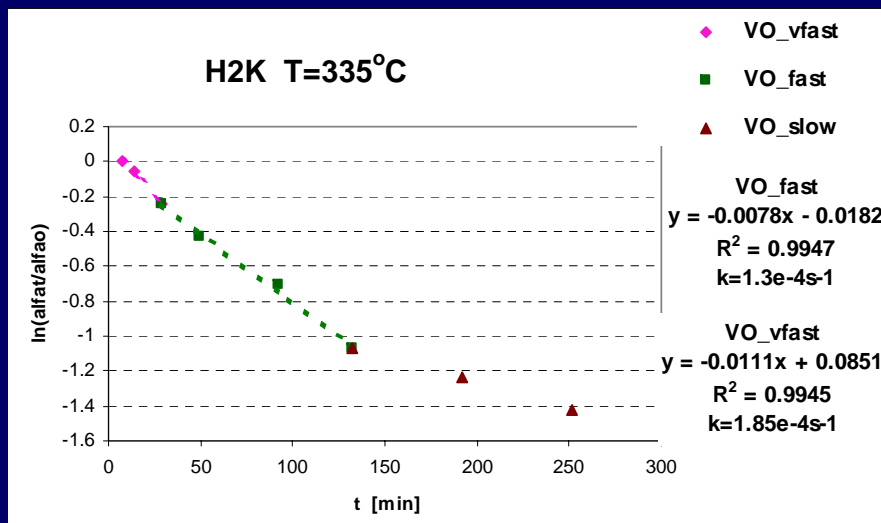
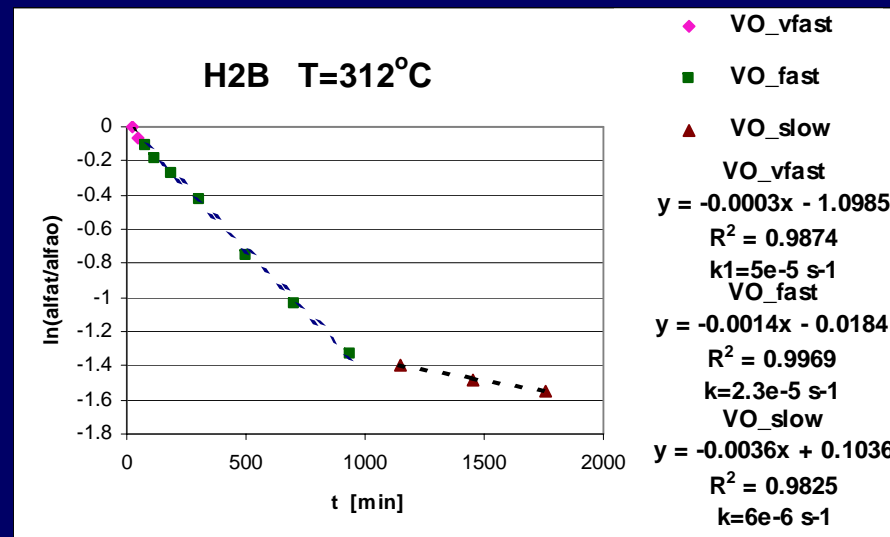
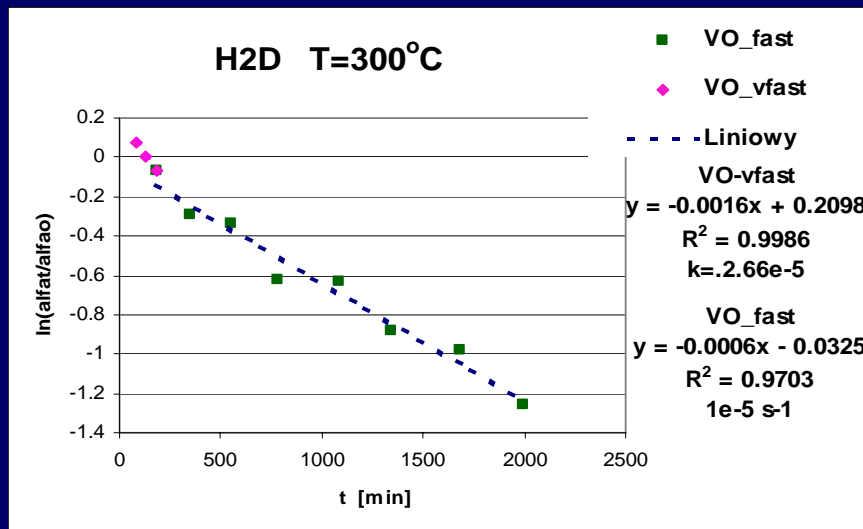
Logarithmic plots of normalised absorption coefficient for **VO** versus time of annealing at 325°C for the samples with different carbon concentration





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Logarithmic plots of normalised absorption coefficient for VO versus time of annealing for the samples from H2 crystal at different temperature

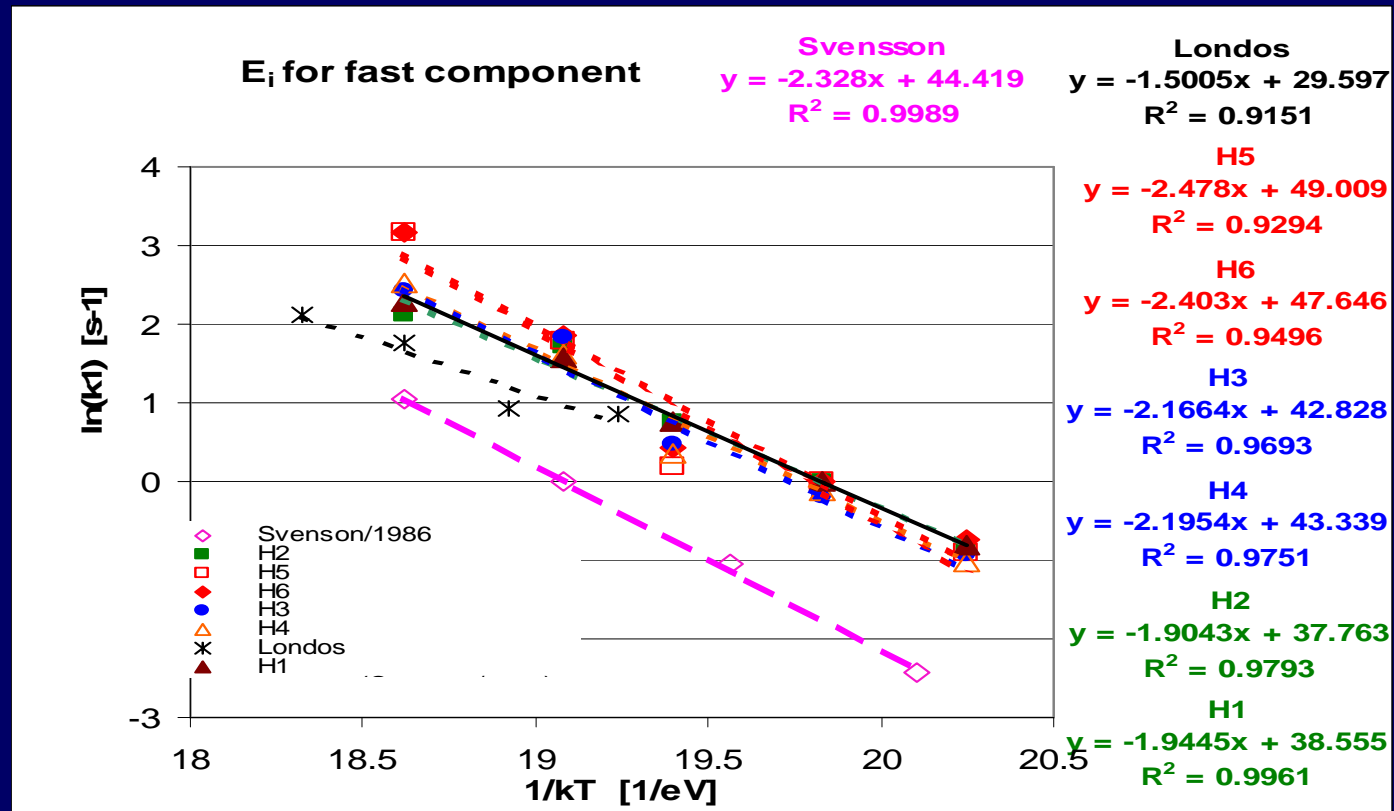




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Arrhenius plots for the fast component of the annihilation of VO defects

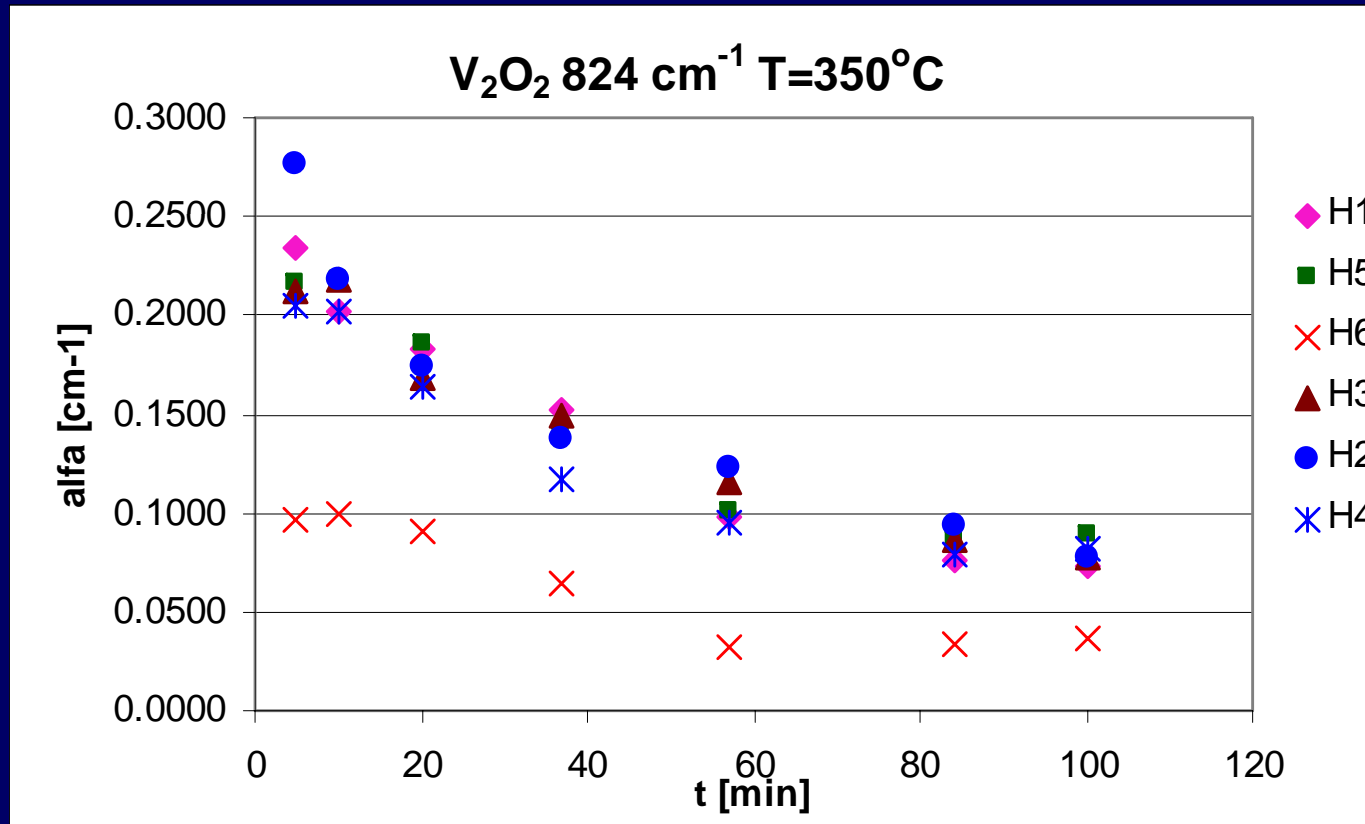
Effect of carbon concentration on the activation energy of the annihilation process of VO complexes



B. Svensson and J. L. Lindström: Phys. Rev. B34, (1986), 870,

C. A. Londos, N. V. Sarlis, L. G. Fytros: J. Appl. Phys. V85, (1999), 8074-78.

The intensity of the absorption band at 824 cm⁻¹ related to V₂O₂ defects

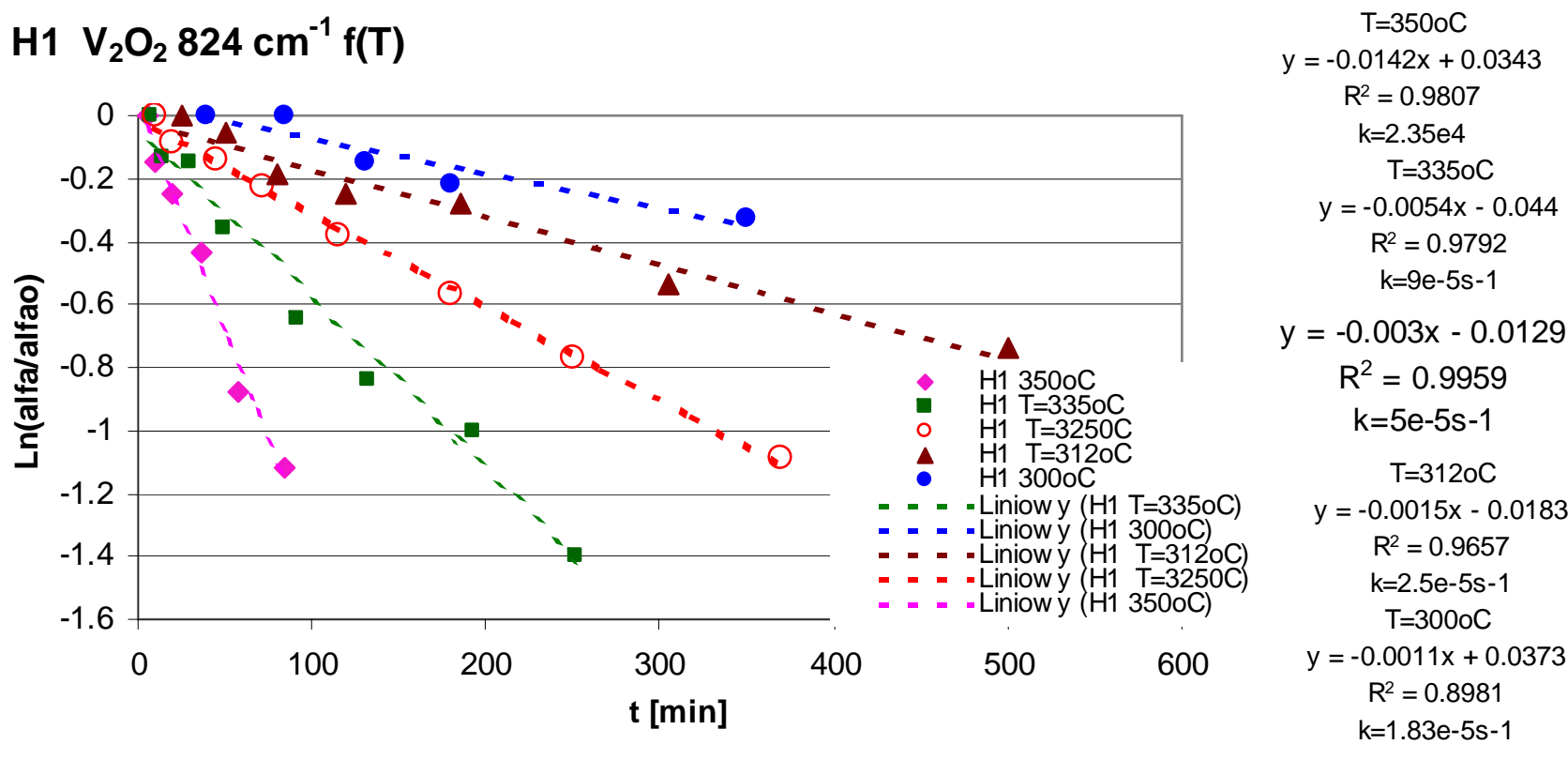




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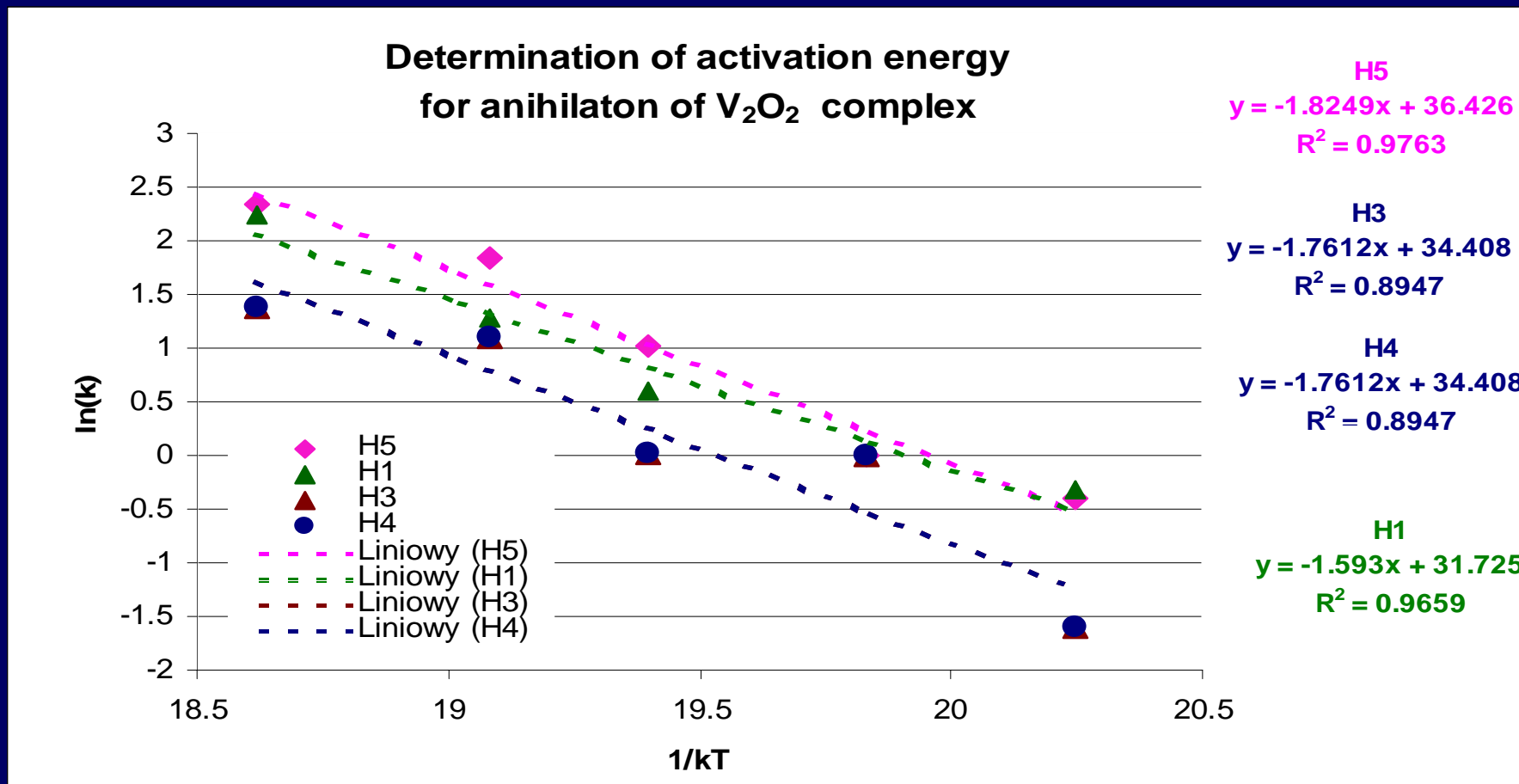
Logarithmic plots of normalised absorption coefficient for V_2O_5 versus time of annealing at various temperatures for the samples from the H1 crystal

H1 V_2O_5 824 cm^{-1} f(T)



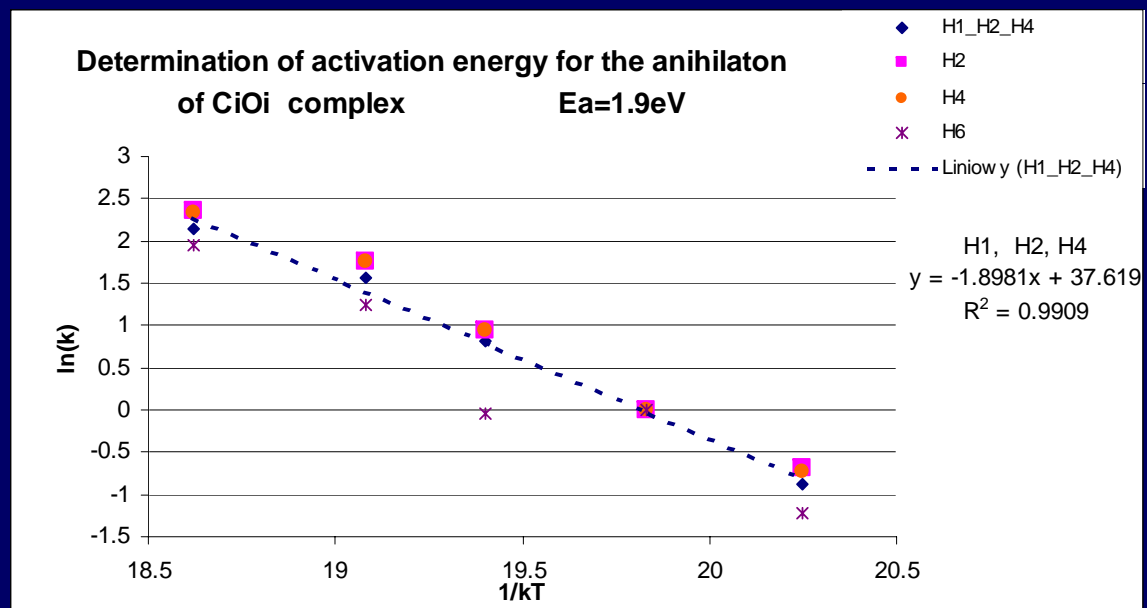
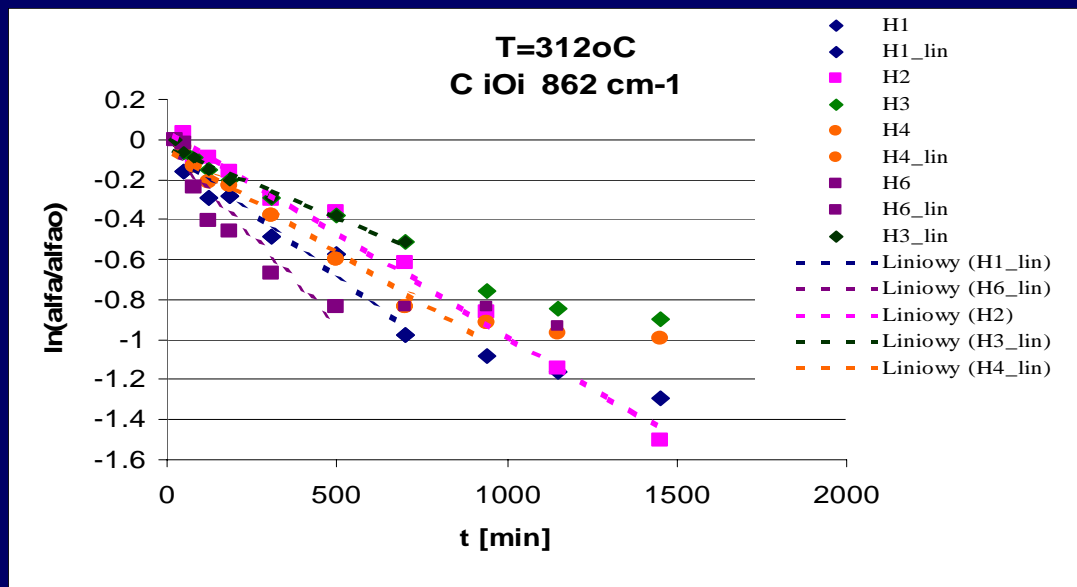


Activation energy for anihilation of V_2O_2 complex





Annihilation of C_iO_i defects



Arrhenius plot
E_a=1.9eV



Multi-reaction model

$k_0=4\pi R(D_{vo}+D_o)$	$VO+O_i \Rightarrow VO_2$	(1)
$k_1=D_d$	$VO \Rightarrow V+O_i$	(2)
$k_2=4\pi R(D_{vo}+D_i)$	$VO+I \Rightarrow O_i$	(3)
$k_3=4\pi R(D_v+D_{O_i})$	$V+O \Rightarrow VO$	(4)
$k_4=4\pi R(D_{vo}+D_v)$	$VO+V \Rightarrow V_2O$	<i>eliminated</i> (5)
$k_5=4\pi R(D_{vo}+D_{vo})$	$VO+VO \Rightarrow VO_2+V$	<i>eliminated</i> (6)
$k_6=4\pi R(D_{CiO_i}+D_v)$	$CiO_i+V \Rightarrow Cs+O_i$	(7)
$k_7=D_{CiO_i \text{ dysoc}}$	$CiO_i \Rightarrow Ci+O_i$	(8)
$k_8=4\pi R(D_{vo_2}+D_o)$	$VO_2+O \Rightarrow VO_3$	(9)
$k_9=4\pi R(D_{Ci}+D_{O_i})$	$Ci+O_i \Rightarrow CiO_i$	(10)



Reaction kinetics

$$d(\text{VO})/dt = -4\pi R(D_{\text{vo}} + D_{\text{oi}})[\text{VO}][\text{O}_i] - D_d[\text{VO}] - 4\pi R(D_{\text{vo}} + D_i)[\text{VO}][\text{I}] + 4\pi R(D_v + D_{\text{oi}})[\text{V}][\text{O}_i] - 4\pi R(D_{\text{vo}} + D_v)[\text{VO}][\text{V}] - 4\pi R(D_{\text{vo}})^2$$

$$d(\text{O}_i)/dt = +4\pi R(D_{\text{vo}} + D_i)[\text{VO}][\text{I}] - D_d[\text{VO}] - 4\pi R(D_{\text{vo}} + D_{\text{oi}})[\text{VO}][\text{O}_i] + 4\pi R(D_v + D_{\text{oi}})[\text{V}][\text{O}_i] + 4\pi R(D_{\text{CiO}_i} + D_v)[\text{CiO}_i][\text{V}]$$

$$d(\text{VO}_2)/dt = +4\pi R(D_{\text{vo}} + D_{\text{oi}})[\text{VO}][\text{O}_i] + 4\pi R(D_{\text{vo}})^2 - 4\pi R(D_{\text{CiO}_i} + D_i)[\text{CiO}_i][\text{I}]$$

$$d(\text{I})/dt = -4\pi R(D_{\text{vo}} + D_i)[\text{VO}][\text{I}] - 4\pi R(D_{\text{CiO}_i} + D_i)[\text{CiO}_i][\text{I}]$$

$$d(\text{V})/dt = +D_d[\text{VO}] + 4\pi R(D_v + D_{\text{oi}})[\text{V}][\text{O}_i] - 4\pi R(D_{\text{vo}} + D_v)[\text{VO}][\text{V}] + 4\pi R(D_{\text{vo}})^2 - 4\pi R(D_{\text{CiO}_i} + D_v)[\text{CiO}_i][\text{V}]$$

$$d(\text{V}_2\text{O})/dt = 4\pi R(D_{\text{vo}} + D_v)[\text{VO}][\text{V}]$$

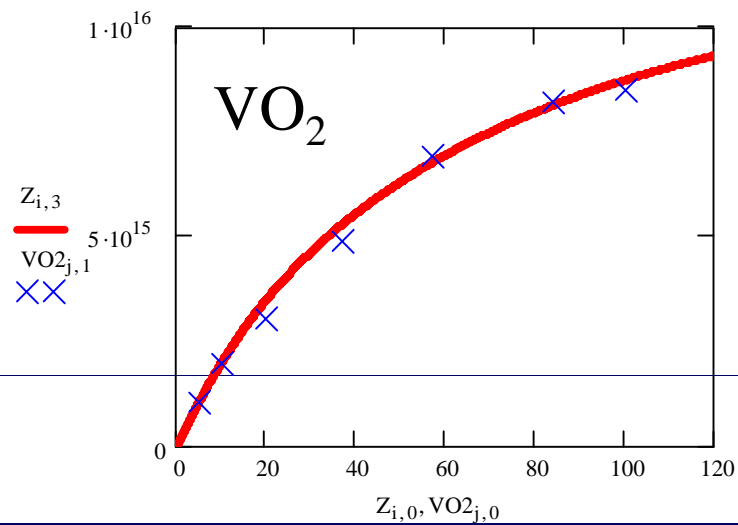
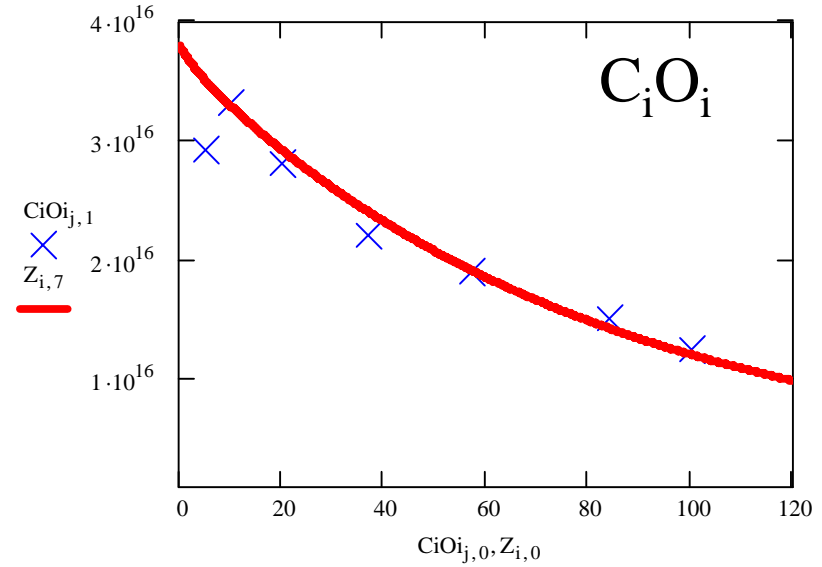
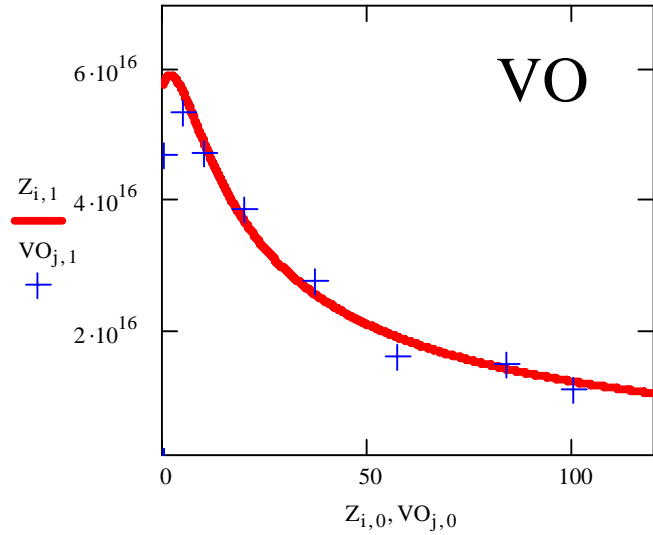
$$d(\text{CiO}_i)/dt = -4\pi R(D_{\text{CiO}_i} + D_v)[\text{CiO}_i][\text{V}] + D_{\text{CiO}_i} \text{dys}^*[\text{CiO}_i] + 4\pi R(D_{\text{Ci}} + D_{\text{O}_i})[\text{Ci}][\text{O}_i]$$

$$d(\text{Ci})/dt = -4\pi R(D_{\text{Ci}} + D_{\text{O}_i})[\text{Ci}][\text{O}_i] + D_{\text{Ci}} \text{dys}^*[\text{CiO}_i]$$



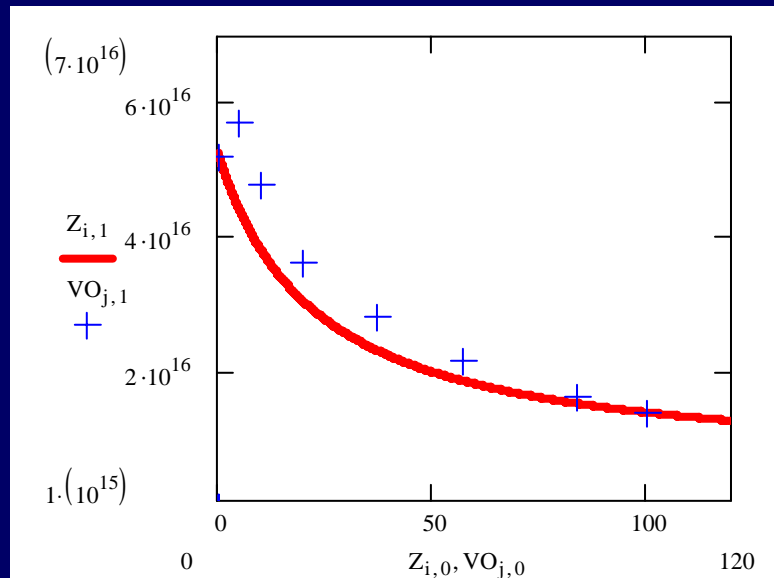
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Fitting results

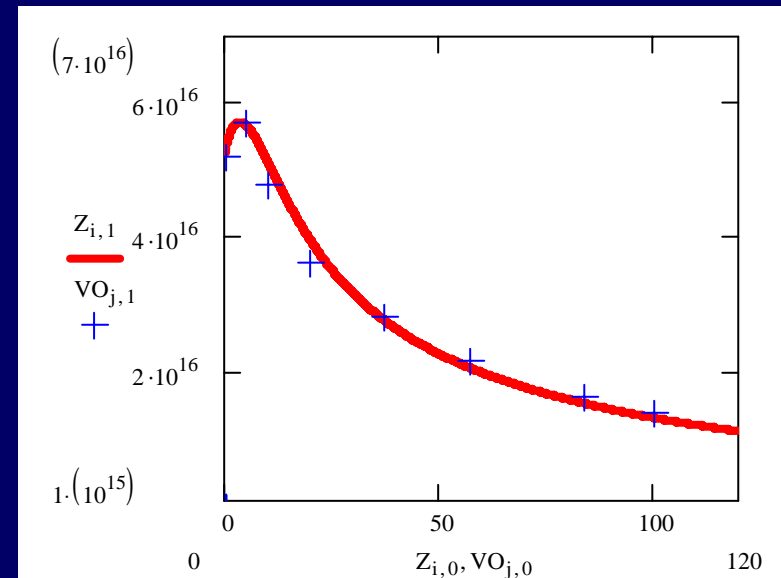




The role of $V+O=VO$ reaction



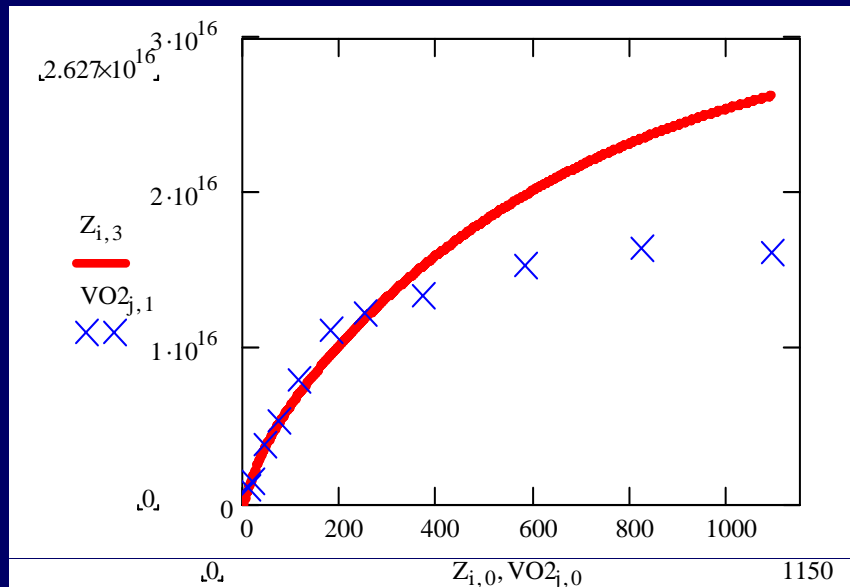
Not considered



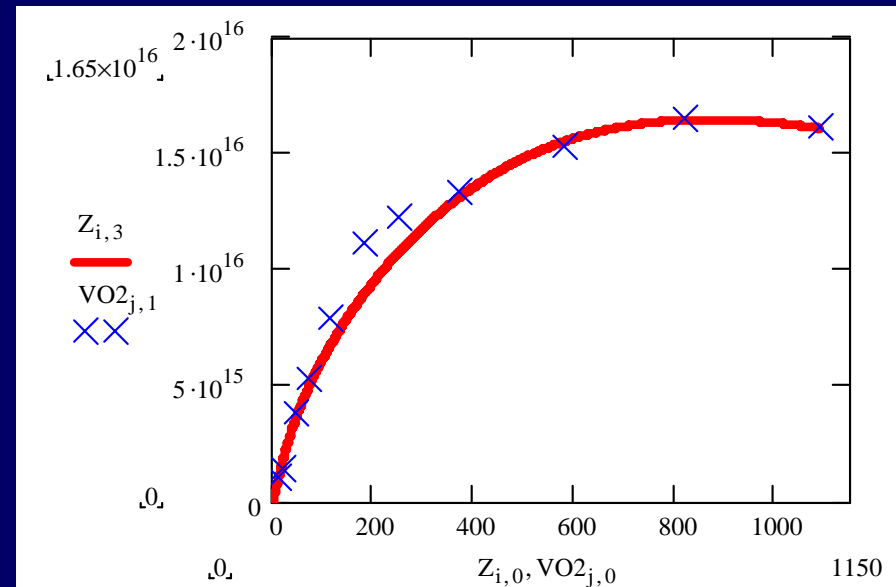
considered



The role of $\text{VO}_2 + \text{O} = \text{VO}_3$ reaction



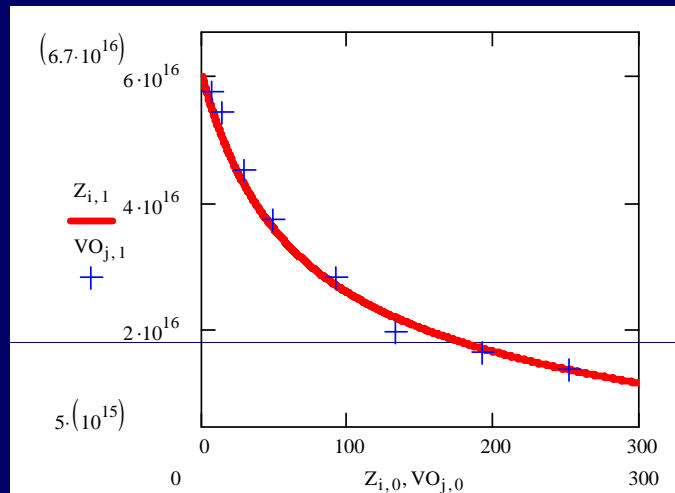
Not considered



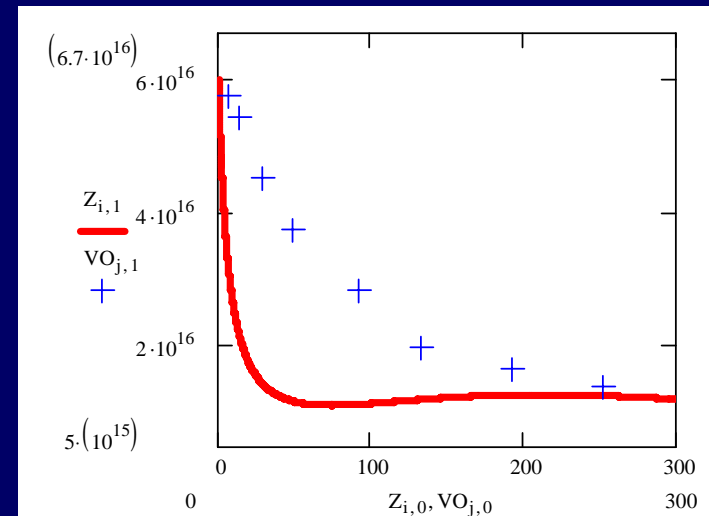
considered



Effective diffusion coefficient for I



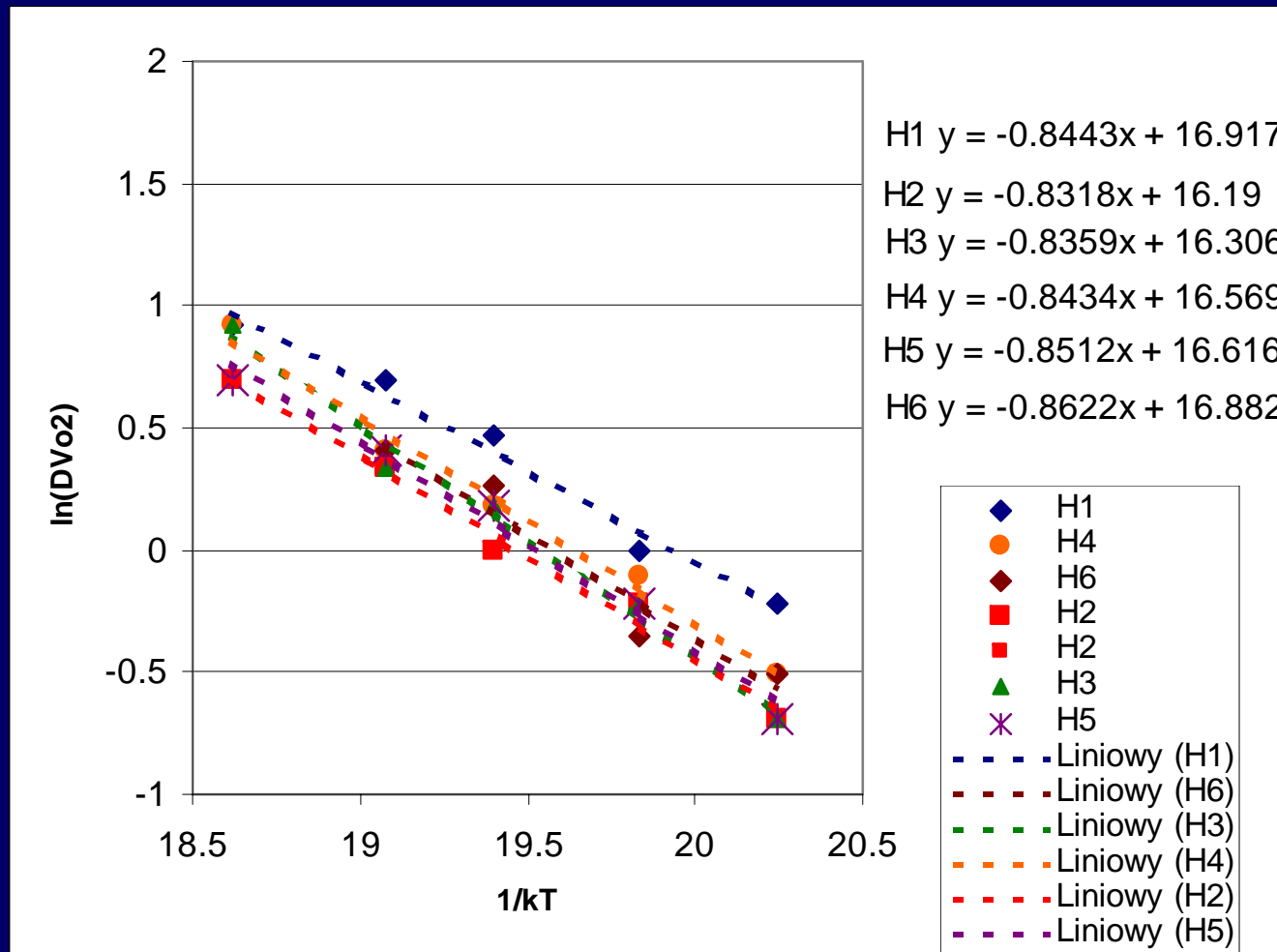
$$D_I = 3.8 \cdot 10^{-14} \text{ cm}^2/\text{s}$$



$$D_I = 3.8 \cdot 10^{-13} \text{ cm}^2/\text{s}$$

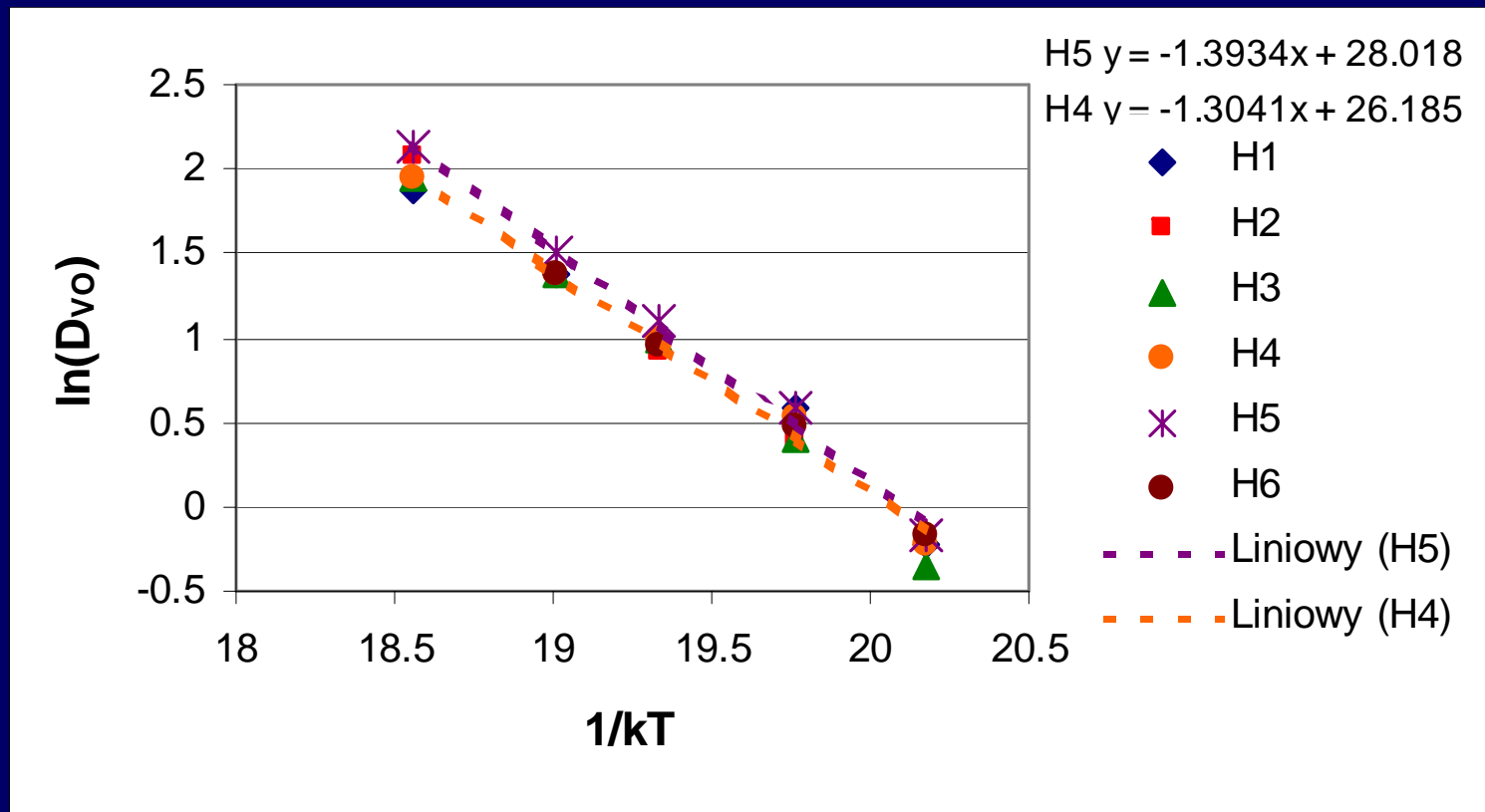


Activation energy for diffusion coefficient D for VO₂ defects



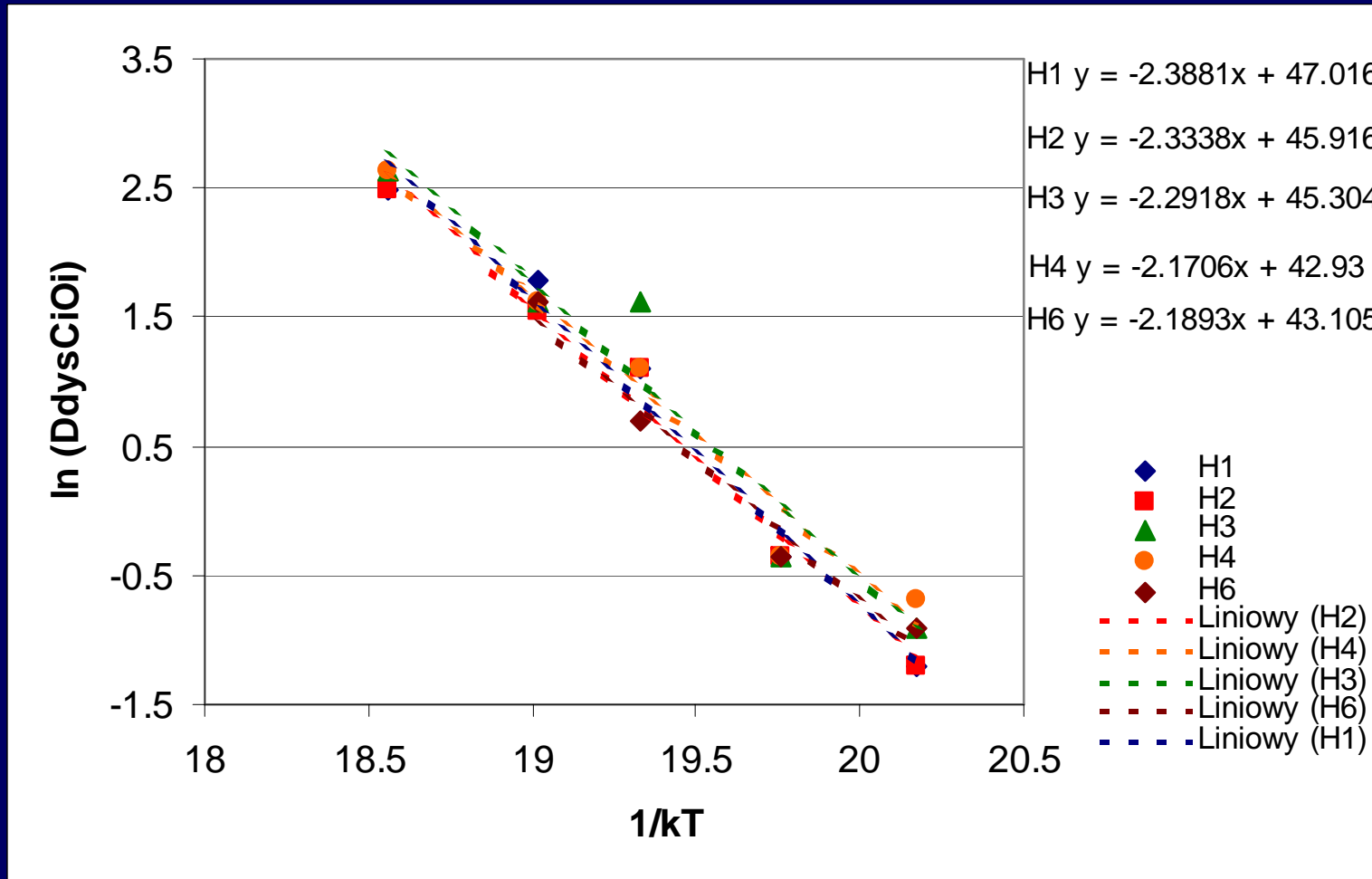


Activation energy for diffusion of VO complex





Activation energy for dissociation of C_iO_i defects





Conclusions (1)

- The kinetic studies of formation and annihilation of complex defects involving oxygen and carbon atoms for the neutron irradiated silicon with enhanced carbon concentration have been performed.
- The concentrations of the defects were calculated from the intensity of the FTIR absorption measurements.
- The temperature dependences of the reaction rate constants have been determined and activation energies for annihilation of V_2O_2 and C_iO_i defects have been found to be 1.7 eV and 1.9 eV, respectively
- An effect of the carbon concentration on the reaction rate constants for the annihilation of VO defect has been observed. The increase of the carbon concentration resulted in decreasing the activation energy of the annihilation process



Conclusions (2)

➤ A multi-reaction model has been used for the fitting the experimental data. The fitting procedure allowed to determine :

- the activation energies for diffusion of VO and VO₂ complexes approximately equal to 1.35eV and 0.84 eV, respectively,
- the activation energy for dissociation of C_iO_i complex approximately equal 2.3 eV.



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Acknowledgements:

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Diffusion coefficient of V and I

According to Sinno D_V , D_I are expressed by the formulas:

$$D_V = 1 \cdot 10^{-3} \exp(-0.457/kT) \text{ i } D_I = 0.242 \exp(-0.937/kT)$$

So at $T=350^\circ\text{C}$ $D_V=2.035 \cdot 10^{-7} \text{ cm}^2/\text{s}$ and $D_I=6.53 \cdot 10^{-9} \text{ cm}^2/\text{s}$.

T. Sinno, R. A. Brown, W. Von Ammon, E. Dornberg ,
Appl.Phys.Lett. V70(17) 2250-2252, 1997



Dissociation

Dissociation process

$$-\frac{\partial [N]}{\partial t} = D_{dys} * [N]$$

D_{dys} –rate constant for dissociation



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The range of uncertainty for fitting parameters

	at/cm ³	at/cm ³	at/cm ³	at/cm ³	at/cm ³									
	[VO]	[O]	[I]	[V]	[CiOi]	D _{VO}	D _O	D _I	D _V	D _{VO2}	D _{dysCiOi}	D _{CiOi}	D _{dysVO}	D _{Ci}
	*10 ¹⁶	*10 ¹⁷	*10 ¹⁶	*10 ¹⁶	*10 ¹⁶	*10 ⁻¹⁶	*10 ⁻²²	*10 ⁻¹⁴	*10 ⁻¹⁵	*10 ⁻¹⁶	*10 ⁻³	*10 ⁻¹⁴	*10 ⁻⁴	*10 ⁻¹⁵
300oC	5.76	8.77	3.5	2	3.5	0.85	5	0.3	0.2	0.7	0.5	0.05	4	0.01
300oC	5.76	8.77	3.5	1	3.5	0.85	5	0.3	0.2	0.7	0.5	0.05	0.4	0.01
300oC	5.76	8.77	6	4.5	3.5	0.85	5	0.45	0.2	0.8	0.4	0.1	0.4	0.01
312oC	5.76	8.77	7	10	3.8	1.8	5	0.8	0.09	0.9	0.6	0.25	0.4	0.1
312oC	5.76	8.77	7	10	3.8	1.8	5	0.8	0.12	1	0.6	0.25	4	0.1
325oC	5.76	8.77	7.5	5.2	3.8	2.7	5	10	15	1.6	3	1.5	4	0.1
325oC	5.76	8.77	7.5	5.2	3.8	2.7	5	10	15	1.6	3	1.5	0.4	0.1
312oC	5.56	9.88	6	6.5	4.5	1.5	5	0.5	0.1	0.8	0.7	0.1	4	0.01
312oC	5.56	9.88	5	4.5	4.5	1.5	5	0.7	0.2	0.8	0.8	0.2	4	0.01
325oC	5.6	9.88	8	6.5	4.6	2.5	5	8	10	1	3	1.5	4	0.1
325oC	5.6	9.88	8.5	7.5	4.6	2.5	5	8	7	1.1	2.5	1.5	4	0.1
325oC	2.2	1.80	3	1.1	1.1	2.6	5	20	20	1.3	2	0.7	4	0.12
325oC	2.2	1.80	6.8	6	0.96	3.8	5	3.5	0.7	1.3	1.9	0.4	4	-
335oC	1.7	2.00	7.2	5.9	0.7	4	5	45	80	1.5	0.8	1.2	4	0.1
335oC	1.7	2.00	6.9	5.8	0.7	4	5	45	80	1.5	5	1.2	4	0.1



Fitting Parameters

TABLE II															
Fitting parameters															
Sample	Temperature [°C]	at/cm ³	at/cm ³	at/cm ³	at/cm ³	at/cm ³	cm ² /s	cm ² /s	cm ² /s	cm ² /s	cm ² /s	s ⁻¹	cm ² /s	s ⁻¹	cm ² /s
		[VO]	[O]	[I]	[V]	[CiOi]	D _{VO}	DO	D _I	D _V	D _{VO2}	D _{dysCiOi}	D _{CiOi}	D _{dysVO}	D _{Ci}
		*10 ¹⁶	*10 ¹⁷	*10 ¹⁶	*10 ¹⁶	*10 ¹⁶	*10 ⁻¹⁶	*10 ⁻²²	*10 ⁻¹⁴	*10 ⁻¹⁵	*10 ⁻¹⁶	*10 ⁻³	*10 ⁻¹⁴	*10 ⁻⁴	*10 ⁻¹⁵
H1	300	5.76	8.77	6	5.5	3.5	0.8	5	0.4	0.2	0.8	0.3	0.1	4	0.01
	312	5.76	8.77	7	10	3.8	1.8	5	0.8	0.12	1	0.6	0.25	4	0.1
	325	5.76	8.77	7.5	5.4	3.8	2.7	5	10	8	1.6	3	1.5	4	0.1
	335	5.76	8.77	9.5	6.5	3.8	4	5	11	12	2	5.5	1	4	0.1
	350	5.76	8.77	6	2	3.8	6.5	5	15	25	2.5	12	1.5	4	0.1
H2	300	5.56	9.88	2.4	2	4.5	0.85	5	0.7	0.7	0.5	0.4	0.4	4	0.01
	312	5.56	9.88	6	6.5	4.5	1.5	5	0.5	0.1	0.8	0.7	0.1	4	0.01
	325	5.6	9.88	8	6.5	4.6	2.5	5	8	10	1	3	1.5	4	0.1
	335	5.56	9.88	10	8	4.5	4	5	10	9	1.4	4.5	1.2	4	0.1
	350	5.26	9.88	6	3	4.6	7	5	15	35	2	13	1.0	4	0.1
H3	300	5.6	8.70	5	4.3	3.2	0.7	5	0.7	0.7	0.5	0.4	0.6	4	0.01
	312	5.8	8.70	6	4.5	1.5	1.5	5	0.5	0.1	0.8	0.7	0.1	4	0.02
	325	5.37	8.70	7.3	5	1.8	2.7	5	10	10	1.2	5	1.5	4	0.1
	335	5.37	8.70	10	8	2.2	4	5	10	9	1.4	4.5	1.2	4	0.1
	350	5.4	8.70	6	2.3	2	7	5	12	50	2.5	14	1.5	4	0.1
H4	300	5.4	9.00	5	4.8	3.01	0.8	5	0.7	0.4	0.6	0.5	0.2	4	0.01
	312	5.4	9.02	6	4.5	3	1.7	5	0.4	0.1	0.9	1.1	0.1	4	0.08
	325	5.4	9.02	7.5	5.8	3.3	2.7	5	12	20	1.4	3	0.7	4	0.12
	335	5.8	9.02	6	3.3	3	4	5	12	15	1.5	5	1.5	4	0.1
	350	5.4	9.02	6	2	2.7	8	5	12	50	2.5	14	1.5	4	0.1
H5	300	5.5	11.00	2.2	2	<1	0.85	5	0.9	0.4	0.5	-	-	4	-
	312	5.1	11.00	4	5	<1	1.7	5	0.7	0.1	0.6	-	-	4	-
	325	5.6	11.00	6.5	5.5	<1	3	5	12;18	15-20	1.2	-	-	4	-
	335	5.3	11.00	6	4.3	<1	5	5	12	15	2.5	-	-	4	-
	350	5.38	11.00	7	4.5	<1	8.5	5	15	20	2	-	-	4	-
H6	300	1.9	2.00	3	1.8	0.9	0.85	5	0.7	0.2	0.6	0.4	0.2	4	0.01
	312	2	2.10	6	6.3	0.8	1.6	5	1.3	0.1	0.7	0.8	0.4	4	0.1
	325	2.2	1.80	3	1.1	1.1	2.6	5	20	20	1.3	2	0.7	4	0.12



SET OF EQUATIONS TO BE SOLVED

$$\begin{aligned}
 d(t, N) := & \left[\begin{array}{l}
 (-k_0 \cdot N_0 \cdot N_1 - k_1 \cdot N_0 - k_2 \cdot N_0 \cdot N_3 + k_3 \cdot N_1 \cdot N_4) \\
 -k_0 \cdot N_0 \cdot N_1 + k_1 \cdot N_0 + k_2 \cdot N_0 \cdot N_3 - k_3 \cdot N_4 \cdot N_1 + k_6 \cdot N_6 \cdot N_4 + k_7 \cdot N_6 - k_8 \cdot N_2 \cdot N_1 \\
 k_0 \cdot N_1 \cdot N_0 - k_8 \cdot N_2 \cdot N_1 \\
 -(k_2 \cdot N_0 \cdot N_3) - (k_8 \cdot N_3) \\
 k_1 \cdot N_0 - k_3 \cdot N_4 \cdot N_1 - k_6 \cdot N_6 \cdot N_4 \\
 k_4 \cdot N_0 \cdot N_4 \\
 -k_6 \cdot N_6 \cdot N_4 - k_7 \cdot N_6 + k_9 \cdot N_7 \cdot N_1 \\
 k_7 \cdot N_6 - k_9 \cdot N_7 \cdot N_1
 \end{array} \right] *
 \end{aligned}$$

$$N := \begin{pmatrix} 5.76 \cdot 10^{16} \\ 8.77 \cdot 10^{17} \\ 0 \\ 6 \cdot 10^{16} \\ 2 \cdot 10^{16} \\ 0 \\ 3.8 \cdot 10^{16} \\ 1 \cdot 10^{16} \end{pmatrix}$$



Deconvolution results

				TABLE II T=300°C										
Sample	thickness	Abs. Line	as irradiated	TX1 300oC/40' abs.coeff. [cm-1]	TX2 300oC/45' abs. coeff [cm-1]	TX3 300oC/45' abs.coeff [cm-1]	TX4 300oC/45' abs.coeff. [cm-1]	TX5 300oC/170' abs.coeff. [cm-1]	TX6 300oC/200' abs.coeff. [cm-1]	TX7 300oC/235' abs.coeff. [cm-1]	TX8 300oC/300' abs.coeff. [cm-1]	TX9 300oC/250' abs.coeff. [cm-1]	TX10 300oC/345' abs.coeff [cm-1]	TX11 300oC/315' abs.coeff. [cm-1]
Total time [min]			0	40	85	130	180	350	550	785	1085	1335	1680	1995
1/T														
H1K	0.197	V ₂ O ₅ _824		0.2768	0.2929	0.2538	0.2366	0.2119	0.2000	0.1815	0.1300	0.1648	0.1368	0.1532
od TX2	0.186	VO_830	0.5762	0.5560	0.5482	0.5035	0.4822	0.4227	0.3414	0.3118	0.2263	0.2114	0.1878	0.1467
		836		0.1295	0.1149	0.1398	0.1413	0.1375	0.1511	0.1367	0.1540	0.1529	0.1593	0.1902
		V ₂ O_839		0.1654	0.1774	0.1613	0.1647	0.1766	0.1839	0.2021	0.1909	0.2215	0.2153	0.2117
H2D	0.2	V ₂ O ₅ _824		0.2672	0.2889	0.2470	0.2510	0.1823	0.1929	0.1680	0.1416	0.1540	0.1211	0.1202
od TX2	0.185	VO_830	0.5556	0.5315	0.5747	0.5329	0.4950	0.3974	0.3805	0.2842	0.2840	0.2198	0.1993	0.1508
		836		0.1236	0.1336	0.1278	0.1336	0.1298	0.1358	0.1824	0.1172	0.1535	0.1574	0.1327
		V ₂ O_839		0.1515	0.1639	0.1638	0.1597	0.1591	0.1840	0.1996	0.2038	0.2160	0.2175	0.1903
H3H	0.202	V ₂ O ₅ _824		0.2315	0.2483	0.2187	0.2230	0.2002	0.1704	0.1448	0.1244	0.1178	0.1068	0.0912
od TX2	0.191	VO_830	0.5369	0.5233	0.5012	0.4764	0.4411	0.3885	0.3304	0.2832	0.2373	0.1911	0.1672	0.1673
		836		0.1121	0.1098	0.1227	0.1174	0.1165	0.1313	0.1154	0.1420	0.1514	0.1430	0.1444
		V ₂ O_839		0.1476	0.1513	0.1498	0.1524	0.1543	0.1647	0.1737	0.1888	0.1895	0.2220	0.2088
H4I	0.202	V ₂ O ₅ _824		0.2274	0.2409	0.2282	0.2194	0.1957	0.1710	0.1554	0.1232	0.1256	0.1152	0.1389
od TX2	0.194	VO_830	0.5380	0.4967	0.4942	0.4815	0.4506	0.4046	0.3579	0.2906	0.2566	0.2319	0.1982	0.1553
		836		0.1386	0.1072	0.1211	0.1150	0.1310	0.1319	0.1365	0.1465	0.1388	0.1399	0.1729
		V ₂ O_839		0.1425	0.1381	0.1484	0.1464	0.1526	0.1711	0.1858	0.2058	0.1957	0.2066	0.2101
H5A	0.215	V ₂ O ₅ _824		0.2394	0.2244	0.2206	0.2075	0.1735	0.1569	0.1423	0.1274	0.1058	0.1120	0.1209
od TX2	0.205	VO_830	0.5087	0.5340	0.5083	0.4818	0.4761	0.3980	0.3764	0.3106	0.2523	0.2215	0.1954	0.1582
		836		0.1201	0.1230	0.4818	0.1053	0.1370	0.1161	0.1243	0.1430	0.1661	0.1350	0.1620
		V ₂ O_839		0.1373	0.1491	0.1490	0.1437	0.1555	0.1653	0.1842	0.1960	0.2132	0.2131	0.1991
H6F	0.2	V ₂ O ₅ _824		0.1101	0.1184	0.1056	0.0951	0.0775	0.0721	0.0702	0.0466	0.0508	0.0415	0.0389
od TX2	0.193	VO_830	0.1808	0.1860	0.1860	0.1498	0.1455	0.1304	0.1008	0.0917	0.0652	0.0560	0.0454	0.0260
		836		0.0727	0.0808	0.0958	0.0899	0.0904	0.0957	0.0941	0.0788	0.0828	0.0849	0.0655
		V ₂ O_839		0.0827	0.0930	0.0883	0.0896	0.0917	0.0896	0.1014	0.0774	0.0853	0.0872	0.0822