Annealing of the vacancy-oxygen and divacancy-oxygen complexes in silicon

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Background

- During irradiation we get:
  - $V + O_i \rightarrow VO$
  - $V + V \rightarrow V_2$

  (V_2 is also produced directly)

- For higher doses:
  - $V + VO \rightarrow V_2O$

  Basis for *I*-level identification

- Another channel for V_2O formation:
  - $V_2 + O_i \rightarrow V_2O$

  Basis for *X*-level identification

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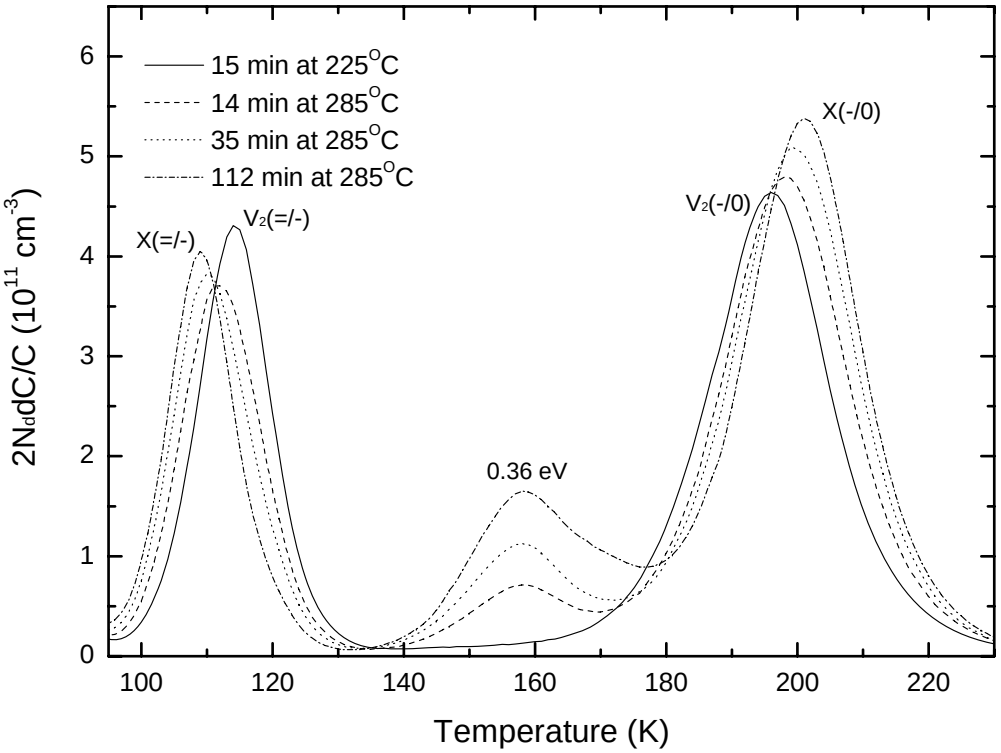
Background



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- X was identified as V_2O
- V_2 migrates:
  - $V_2 + O_i \rightarrow V_2O$

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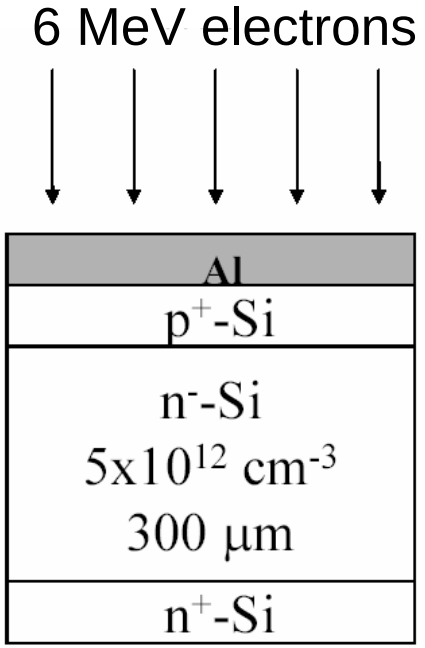
Experiment

Survey of the samples used in the study:

Sample	Doping (P/cm^3)	Carbon (cm^{-3})	Oxygen (cm^{-3})
MCZ-Si	5.5×10^{12}	$\leq 10^{16}$	$(5–10)\times10^{17}$
DOFZ-Si	5.0×10^{12}	$(2–4)\times10^{16}$	$(2–3)\times10^{17}$

- DOFZ = Diffusion-Oxygenated Float-Zone Si
- MCZ = Magnetic Czochralski
- Experimental method:
  - DLTS
  - Pre-annealing to insure a $V_2 \rightarrow V_2O$ transformation.
  - Isothermal annealing in the range 275-355 ^oC.



Dose: 2 - 5 $\times10^{12}$ cm^{-2}

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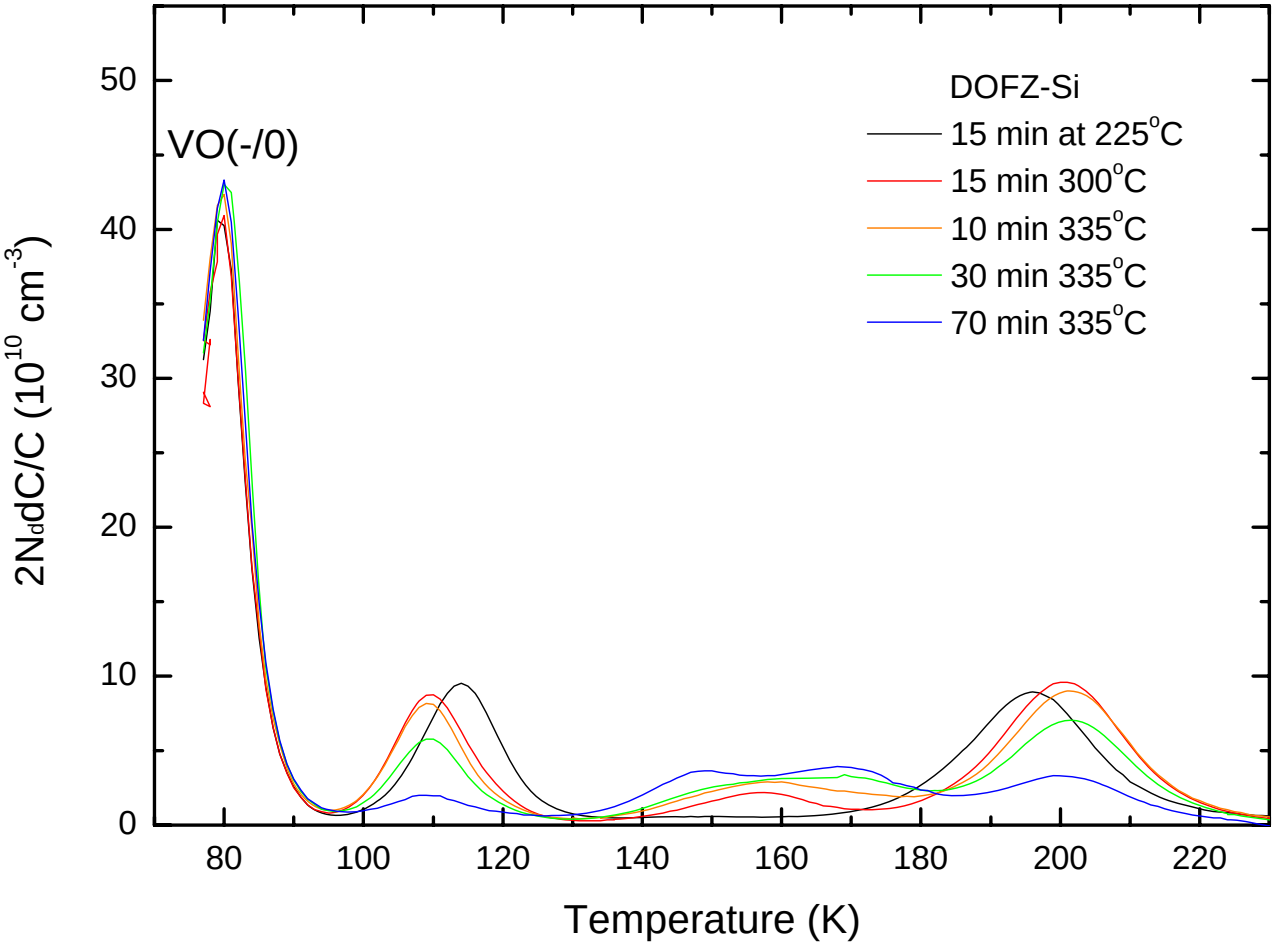
Results: DOFZ - Si



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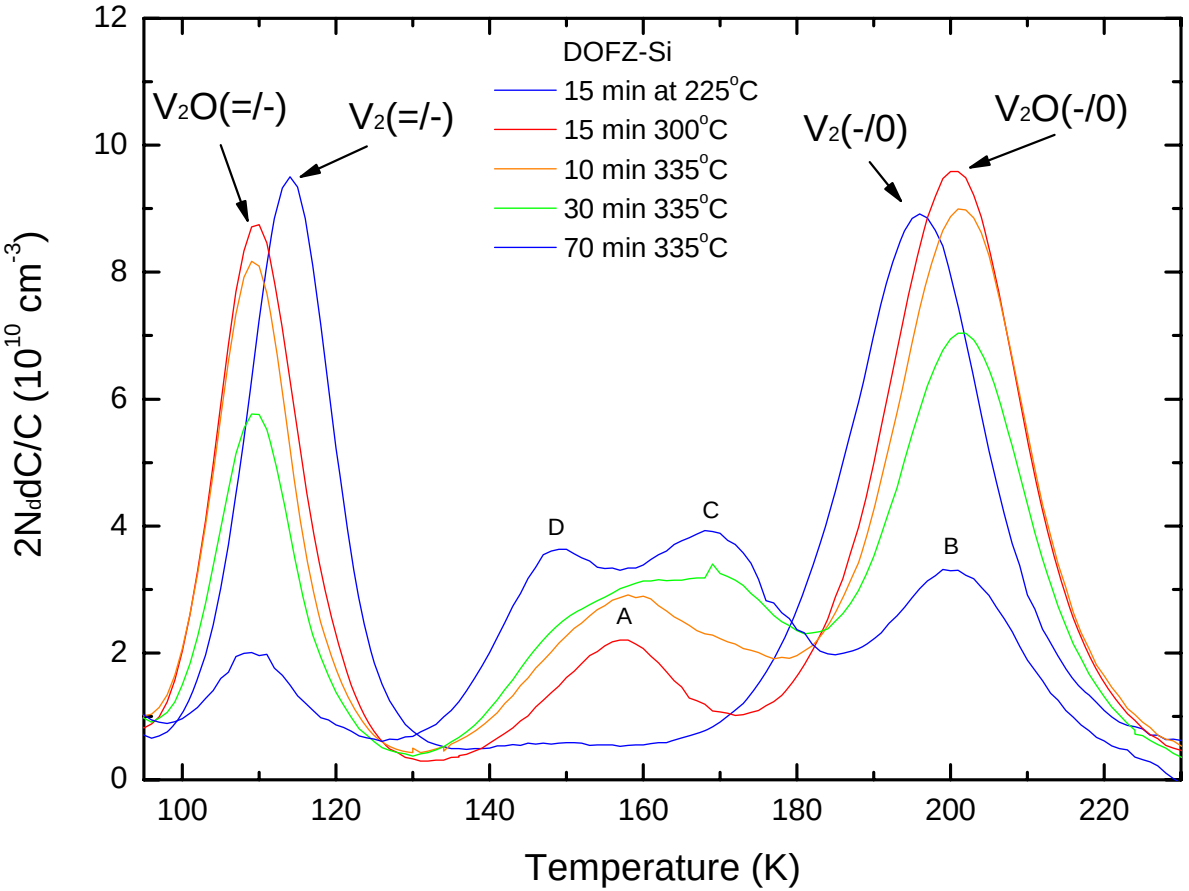
Results: DOFZ - Si



- Other levels observed:
  - A at ~157 K (*)
  - B at ~200 K
    - Similar electrical parameters as $V_2O(-/0)$.
  - C at ~175 K
  - D at ~157 K

(*) To be discussed in:
"*On the formation of the L-center in silicon during heat treatment in the temperature range 205 to 285°C*"
M. Mikelsen, E. V. Monakhov, B. S. Avset, B. G. Svensson
To be published in "Physica sicripta"

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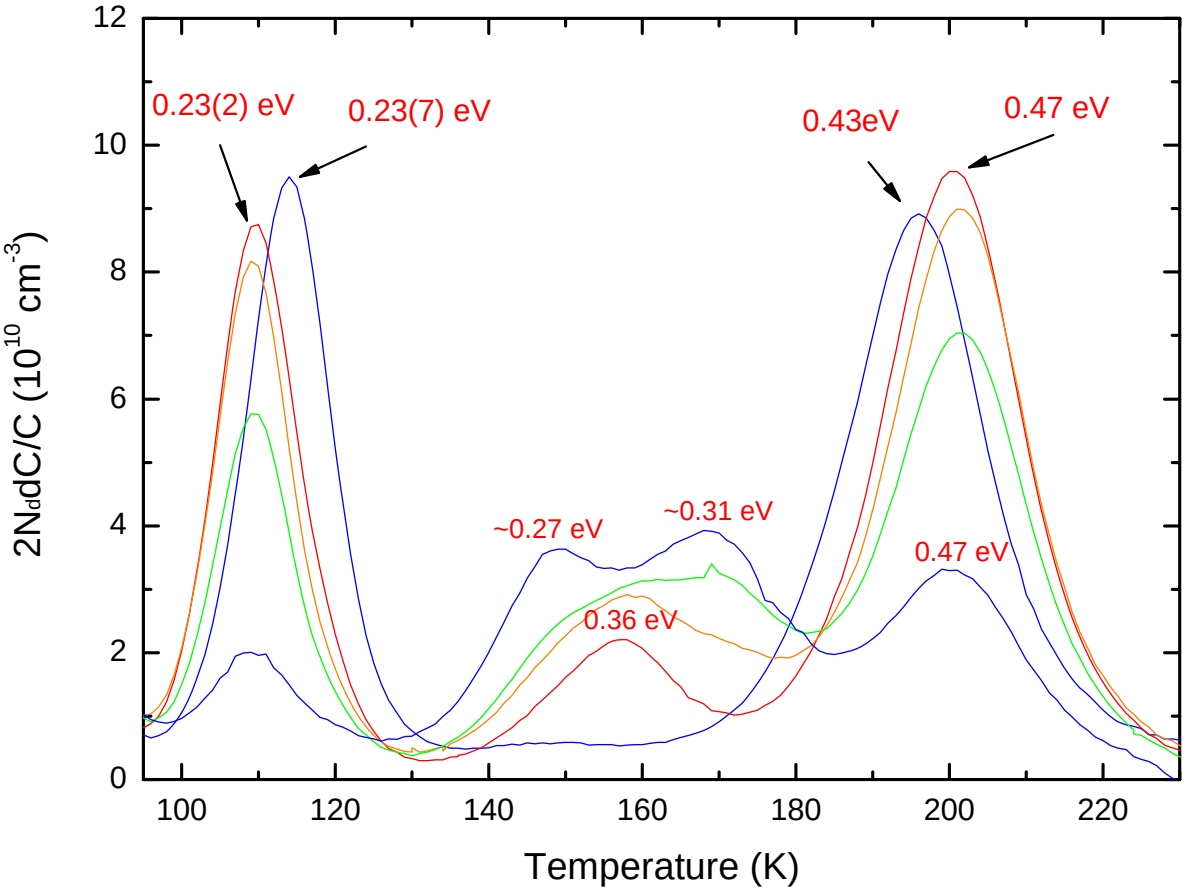
Results: DOFZ - Si



- The activation enthalpies for peak C and D were obtained by using a computer program that fits the spectrum to a sum of single peaks.

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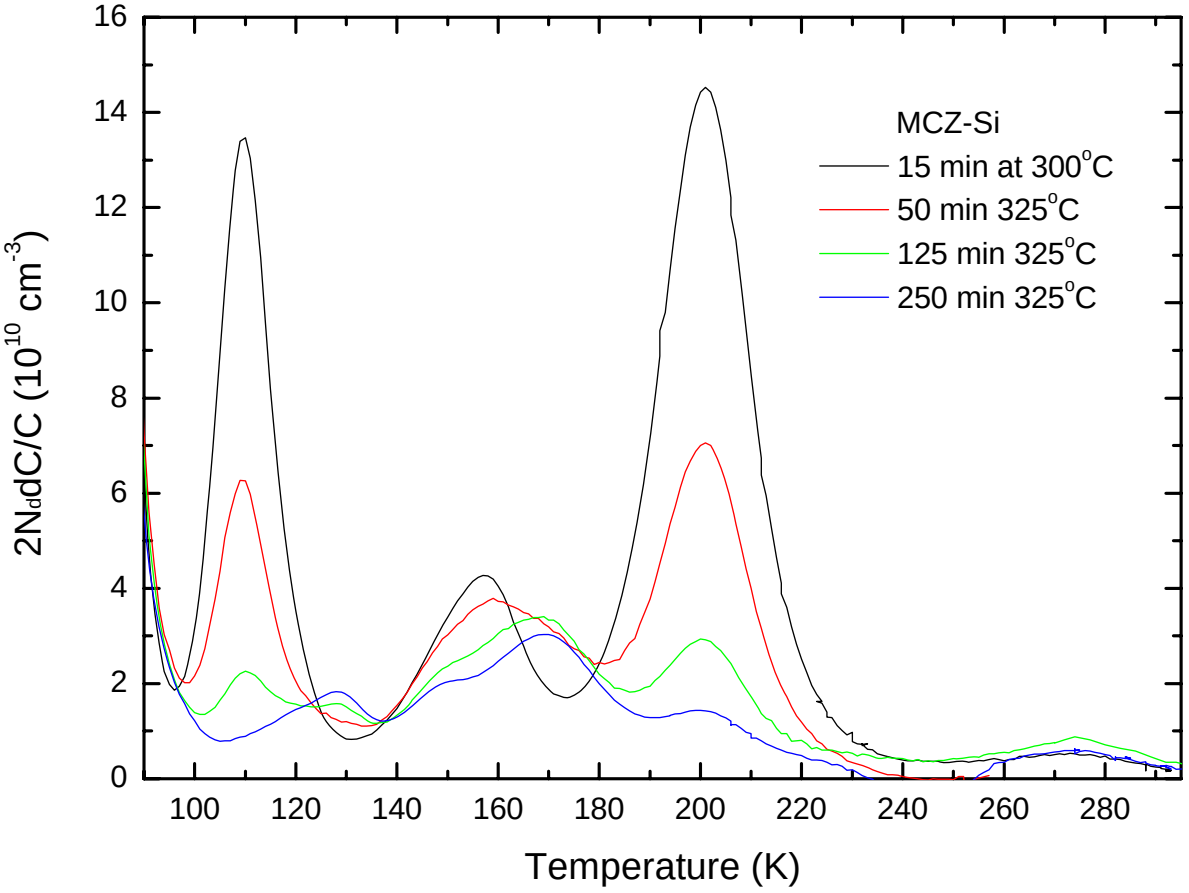
Results: MCZ Si



- MCZ-Si behaves similar to DOFZ
  - But the area between the two V_2O peaks looks a little bit different. (No D-peak)

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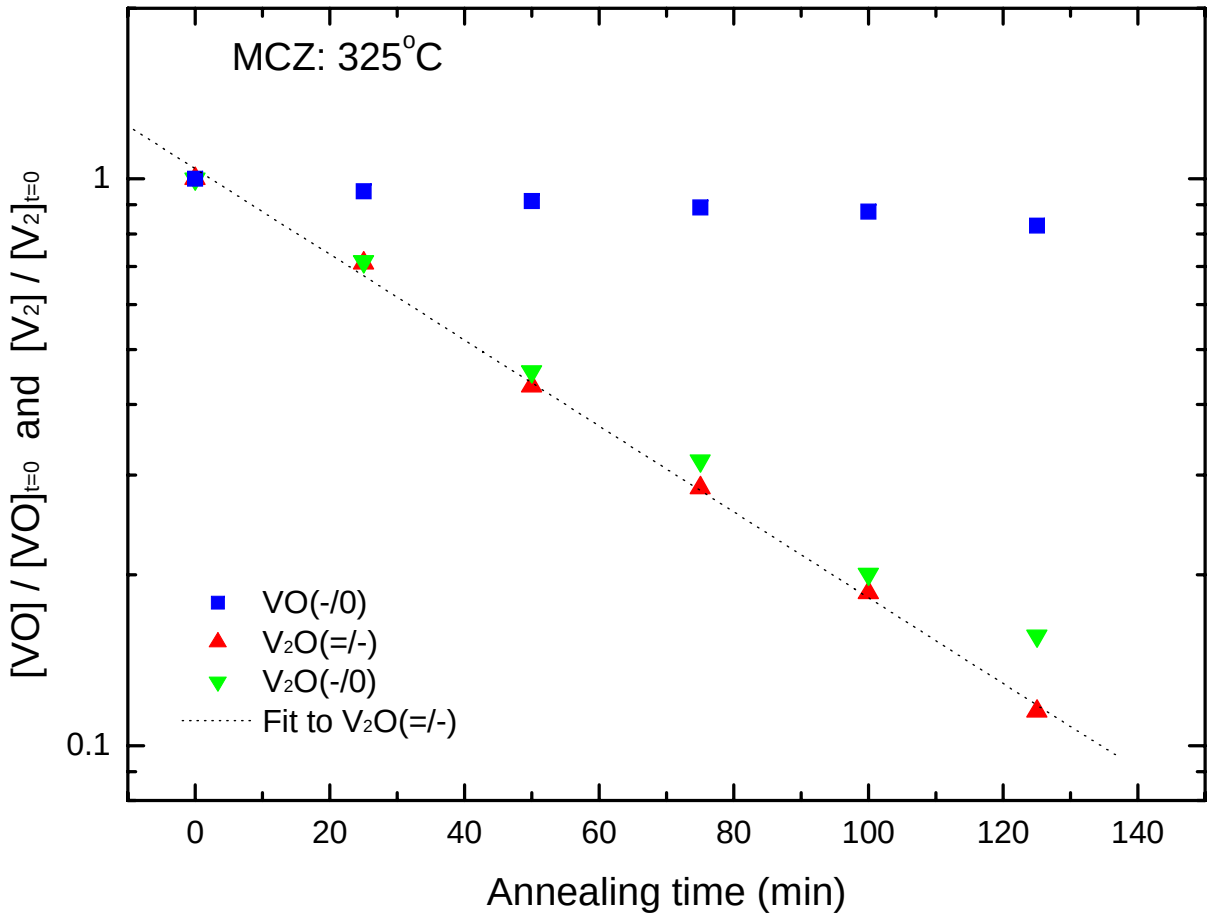
Results: V_2O annealing

Example:



- The annealing of $V_2O(=/-)$ exhibits first order kinetics.
  - For both MCZ and DOFZ.
  - For all annealing temperatures in the range 275 - 355 °C.
  - The kinetics for V2O(-/0) is affected by overlapping level.

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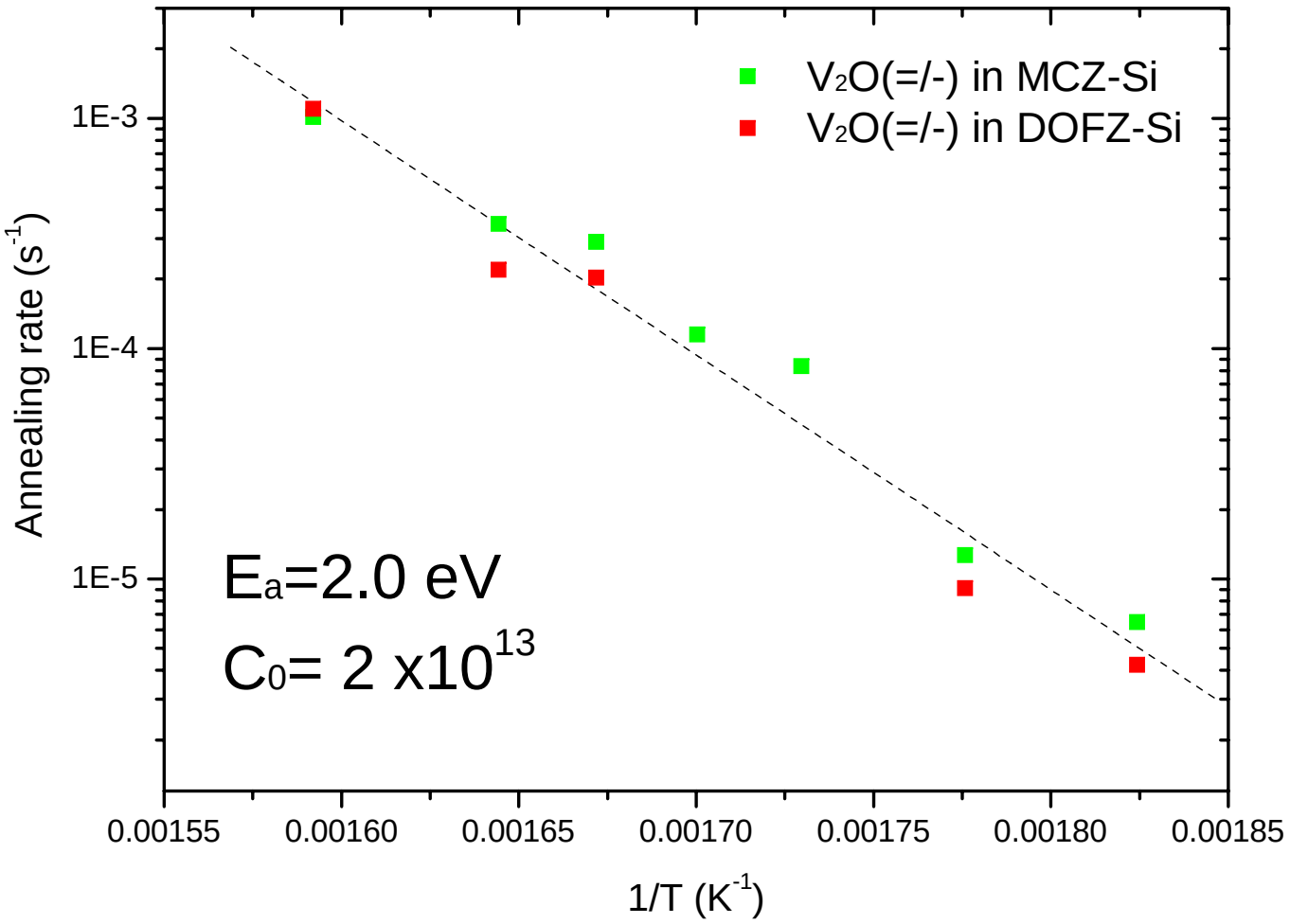
Results: V_2O annealing



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The V_2O annealing mechanism

- It is improbable that V_2O anneals by migration and trapping.
  - Since O_i is the main impurity, one would expect V_2O_2 to form.
  - V_2O_2 is believed to be electrically active with two acceptor centers similar to V_2 and V_2O.
- V_2O does not anneal by interacting with migrating oxygen dimers.
  - The diffusivity of O_2 is to low by a factor 10^4.

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The V_2O annealing mechanism

- A prefactor, c_0, in the 10^{12} – 10^{13} range is expected for dissociation.
  - The experimental value is in this range taking in regard the uncertainty.
  - If dissociation were to occur we would expect an increase in VO;

    $V_2O \rightarrow V + VO$

…. So we must investigate the VO annealing, to check if it really is dissociation.

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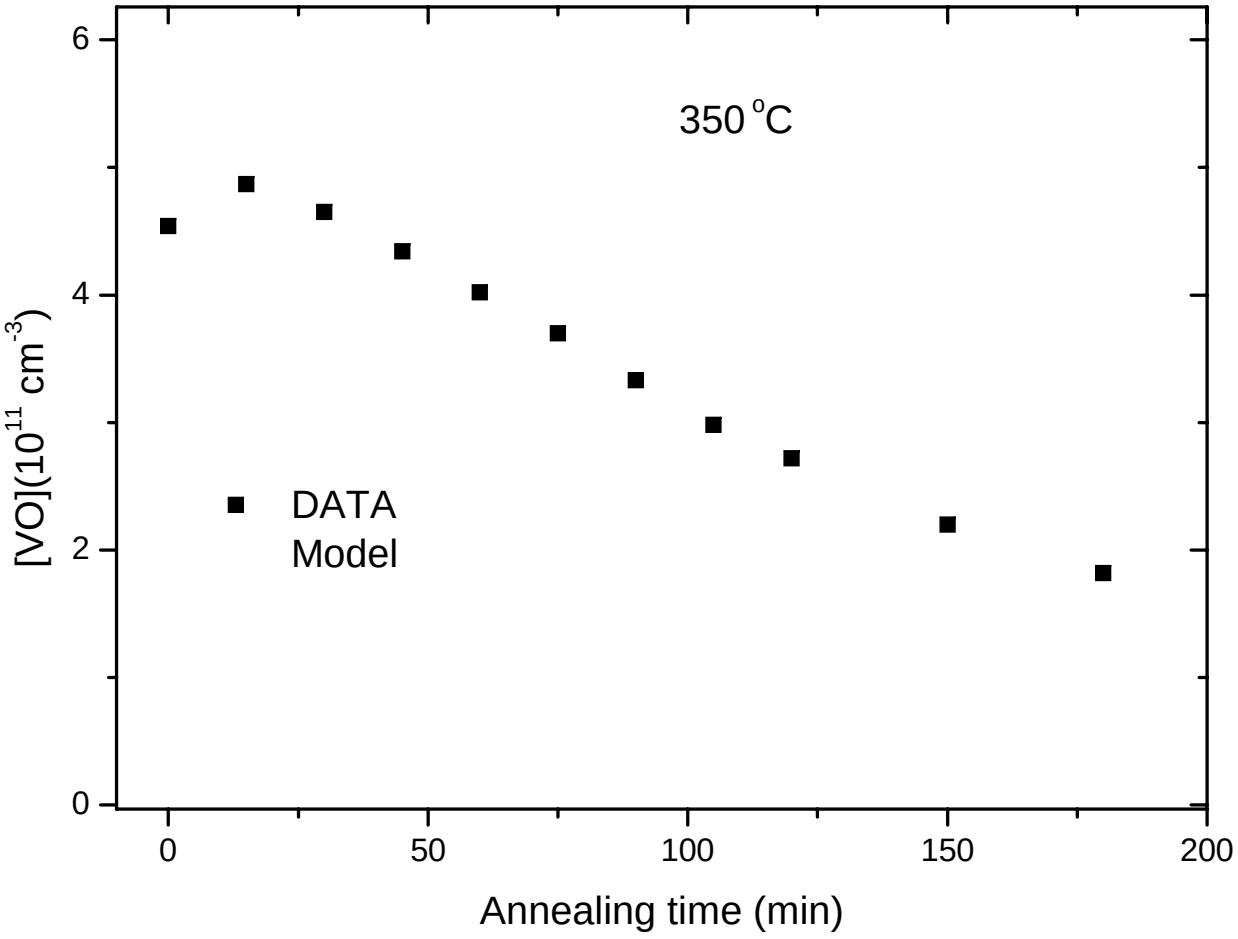
Results: VO annealing (DOFZ)



- After the initial increase, [VO] decreases with 1st. order kinetics.

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A model for defect annealing

- The reactions
  - $V_2O \rightarrow VO + V$ (dissociation)
  - $V + Oi \rightarrow VO$ (migration of V)
  - $VO + Oi \rightarrow VO_2$ (migration of VO)
  - $VO \rightarrow V + O_i$ (dissociation)
  - $VO + V \rightarrow V_2O$ (migration of V)

- The diff-equations
  - $d[VO]/dt = - C_{diss\_V2O}(T)\,[V_2O] + 4\pi R\, D_V(T)\,[V]\,[VO]$
  - $d[VO]/dt = C_{diss\_V2O}(T)\,[V_2O] + 4\pi R\, D_V(T)\,[V]\,[O_i] - 4\pi R\, D_{VO}(T)\,[VO]\,[O_i] - C_{diss\_VO}(T)\,[VO] - 4\pi R\, D_V(T)\,[V]\,[VO]$
  - $d[V]/dt = C_{diss\_V2O}(T)\,[V_2O] + C_{diss\_VO}(T)\,[VO] - 4\pi R\, D_V(T)\,[V]\,[O_i] - 4\pi R\, D_V(T)\,[V]\,[VO]$

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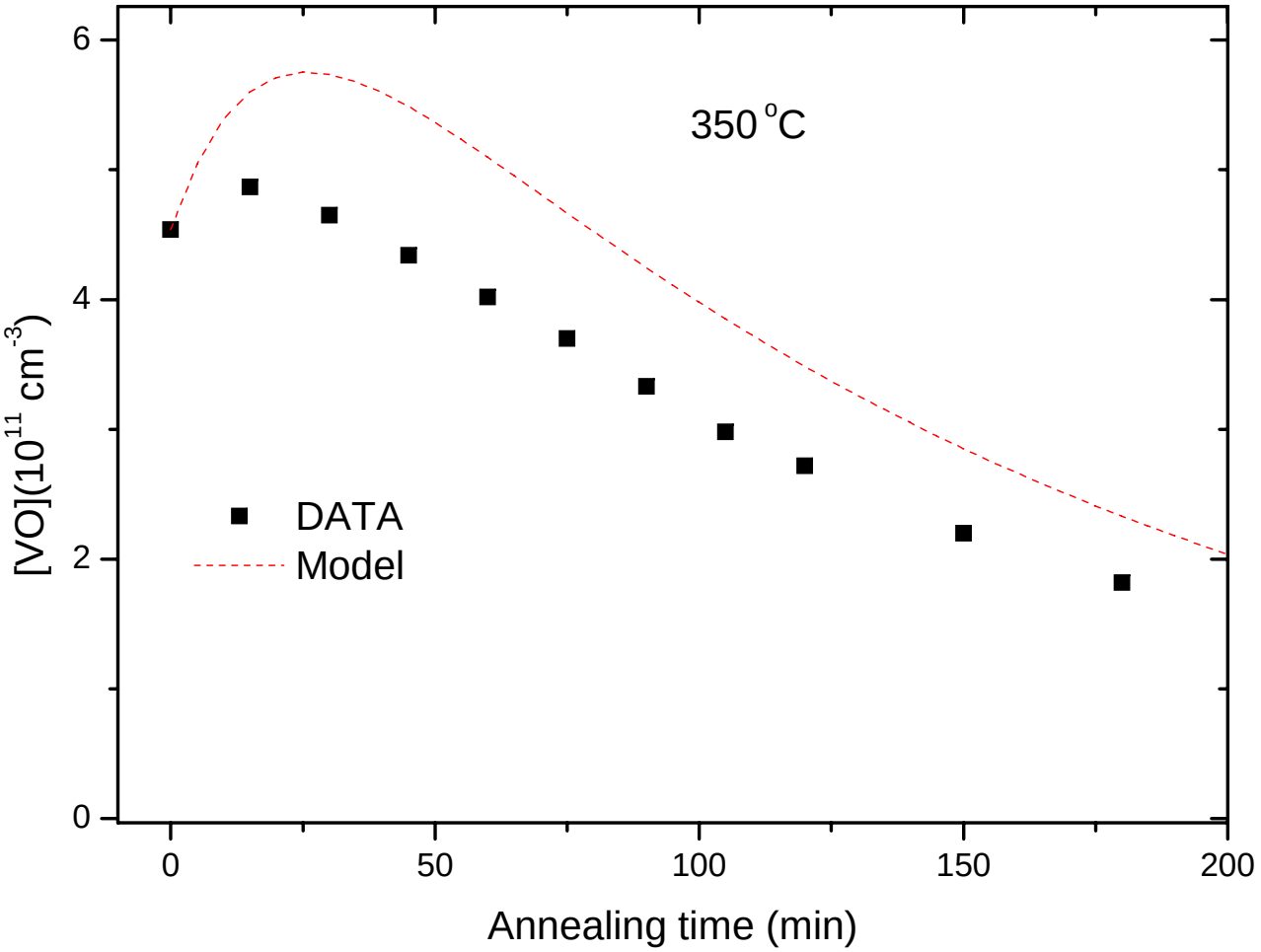
Results: VO annealing (DOFZ)



- The model is highly sensitive to the $[O_i]$ concentration. We used $[O_i]= 2.5 \times 10^{17}$.

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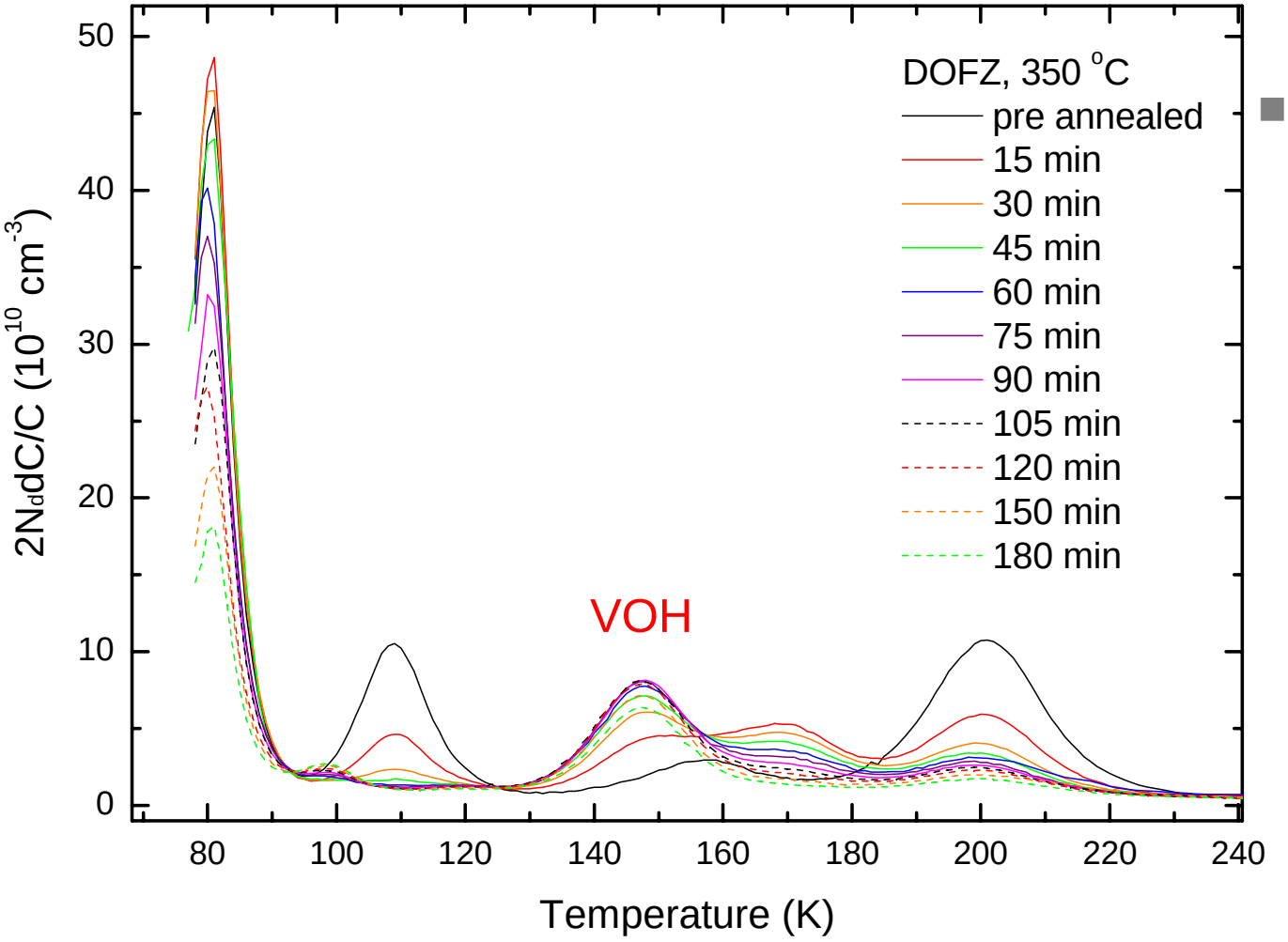
Results



- Hydrogen may interact with VO.

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Summary

- The V_2O defect anneals with an activation energy, E_a, of ~2.0 eV and a prefactor ~2 x 10^{13} s^{-1}.

- Dissociation is the likely annealing mechanism for V_2O.

- A model that includes VO and V_2O dissociation and VO migration and trapping describes the observed annealing kinetics well.

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