UNIVERSIDADE DE AVEIRO

VI Annual Meeting i3N, Lisboa 2017

Powerful recombination centers resulting from reactions of hydrogen with carbon-oxygen defects in solar silicon

P. Santos* and J. Coutinho
Department of Physics & I3N, University of Aveiro, Campus Santiago, 3810-193 Aveiro, Portugal
M. Vaqueiro-Contreras, V. Markevich, M. Halsall, A. R. Peaker,
Photon Science Institute, University of Manchester, M13 9PL, UK

Abstract:

The introduction of Hydrogen has been shown to be an effective method to mitigate the recombination activity of several defects and impurities in solar Si. Nevertheless, we found that, under certain conditions, hydrogen atoms can interact with existing carbon and oxygen, resulting in the formation of powerful recombination centers [1]. Experimental data shows the formation of a dominant COH related center with an acceptor level at E_v+0.36 eV. Here we propose a theoretical model, based on *ab-initio* calculations, that can be assigned to the experimental observation of the aforementioned recombination center. Our model consists in a bi-stable COH defect with two distinct configurations in the neutral and negative charge state. The calculated reconfiguration barrier from the negative to the neutral state configuration is 0.22 eV while the reverse path has virtually no barrier. This should allow for the defect to shift between configurations at room temperature upon capture of charge carriers. We predict an acceptor level for this defect at E_v+0.32 eV in good agreement with experimental observations.

Introduction:

Deep level transient spectroscopy (DLTS) experiments crossed with infrared absorption measurements [1] allowed to assign the formation of two DLTS peaks, labeled as H1/H2, to one or more recombination centers with C, O and H elements in their constitution. The dominant center, related to the H2 peak, produces an acceptor level at E_v+0.36 eV. Here we propose a model of the COH defect that is compatible with the experimental observation and explains the observed acceptor level. We employed the density functional code VASP with the projected augmented wave method [2]. The transformation barriers were calculated with the nudged elastic band method [3]. The electrical levels were calculated with the marker method [4].

Tab1: Energies associated to the steps presented in the diagram of fig. 1 and calculated COH(-/0) level

	S-D-S	S-D'-S
(1)	Electron-hole pair excitation	
(2) $COH_{s\text{-}state}(-/0)$	~E_v+0.01 eV	~E_v+0.01 eV
(3) $\Delta E[(S)^0 \rightarrow (D/D')^0]$	0.22 eV	0.41 eV
(4) $COH_{D/D'\text{-}state}(-/0)$	E_c−0.14 eV	E_c−0.28 eV
(5) $\Delta E[(S)^- \rightarrow (D/D')^0]$	<0.1 eV	0.33 eV
COH(-/0)	E_v+0.32 eV	E_v+0.27 eV

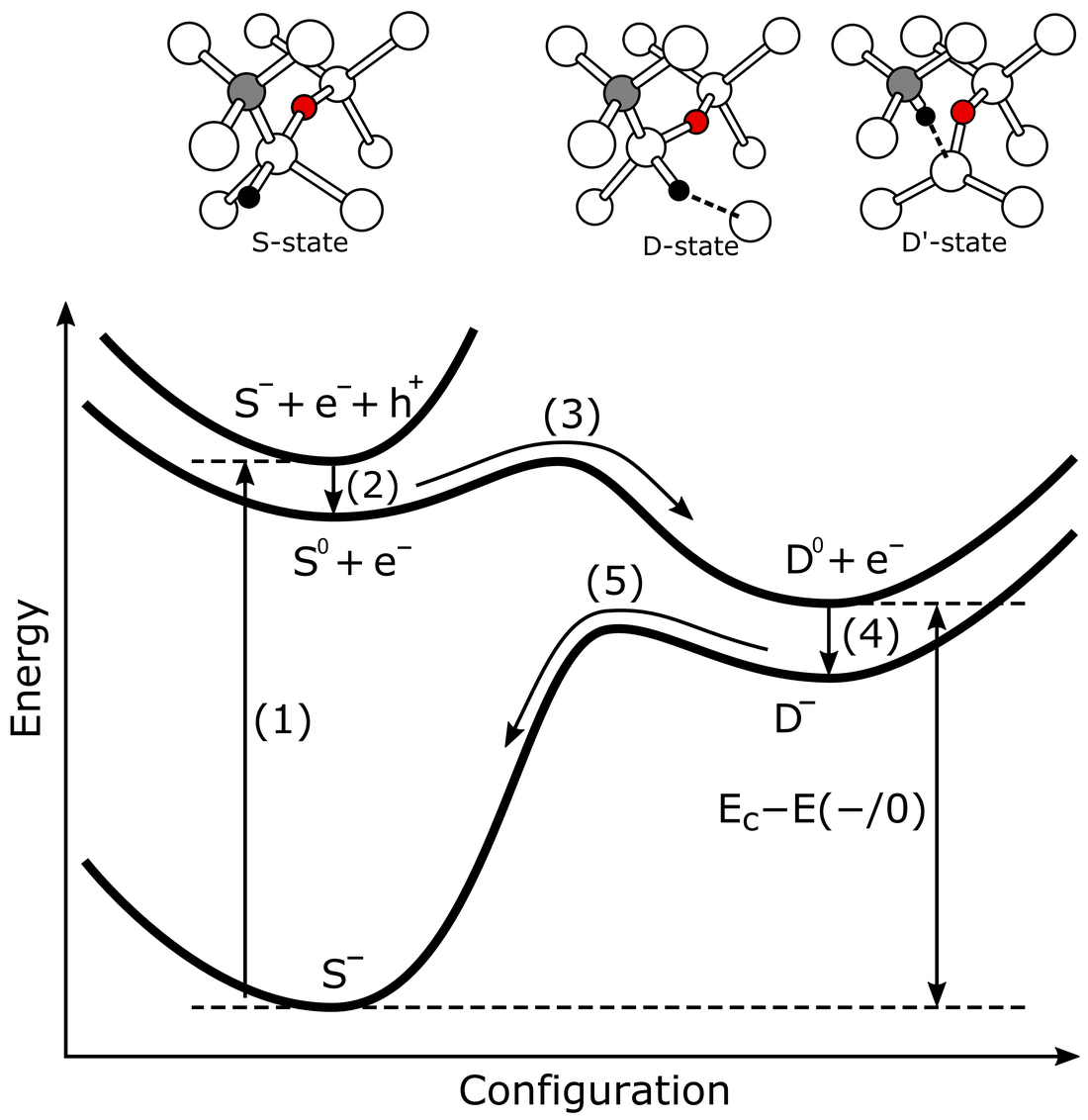

Fig1: Configuration-coordinate diagram of the model proposed to the minority carrier recombination mechanism in solar Si due to a C-O-H complex. C, O, H and Si atoms are shown in gray, red, black and white, respectively.

C-O-H defect re-configuration mechanism:

(1) Photo excitation with the creation of free carriers.

(2) Capture of a hole (minority carrier) by $(S)^-$. When in the S configuration, the COH is a shallow acceptor.

(3) Reconfiguration to the neutral $(D/D')^0$ state. The lowest energy barrier is from $(S)^0$ to $(D)^0$ with a 0.22 eV barrier. D and D' are nearly degenerate in the neutral charge state. Other possible paths are less likely at room temperature (barriers above 1eV)

(4) Capture of an electron (majority carrier). D and D' are *deep* acceptors in the region of 0.1 to 0.3 eV bellow the conduction band.

(5) back-conversion into the $(S)^-$ state. $(D)^-$ to $(S)^-$ has virtually no barrier. Back-conversion barrier from $(D')^-$ is 0.33 eV.

Conclusions:

We proposed a model for the COH defect which explains the measured acceptor level in ref. [1] at E_v+0.36 eV. This level is not explained by the vertical transitions (2) and (4). However, when considering the balance associated to the electron capture of $(D)^0$ and transformation to $(S)^-$ we arrive at an acceptor level at E_v+0.32 eV.
Although the S →D →S path should be dominant due to the lower transormation barriers, the alternative path S →D' →S is also viable at room temperature. This could explain the less dominant DLTS signal H1 observed in ref. [1]

References:

[1] M. Vaqueiro-Contreras, V. Markevich, M. Halsall, A. R. Peaker, P. Santos, J. Coutinho, S. Öberg, L. Murin, R. Falster, J. Binns, E. Monakhov, and B. G. Svensson, to appear in Applied Physics Letters.

[2] G. Kresse and J. Hafner, Phys. Rev. B **47** , 558 (1993)

[3] G. Henkelman, B. P. Uberuaga and H. Jonsson, J. Chem. Phys. **113**, 9901 (2000)

[4] A. Resende, R. Jones, S. Öberg, and P.R. Briddon, Phys. Rev. Lett **82**, 2111 (1999).

This work was funded by the FCT under projects PTDC/CTM-ENE/1973/2012 and UID/CTM/50025/2013, and funded by FEDER funds through the COMPETE 2020 Program. Computer resources were partially provided by the Swedish National Infrastructure for Computing (SNIC) at PDC.

Cofinanciado por:
COMPETE 2020 PORTUGAL 2020 UNIÃO EUROPEIA Fundo Europeu de Desenvolvimento Regional
FCT Fundação para a Ciência e a Tecnologia
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E ENSINO SUPERIOR

INSTITUTE FOR NANOSTRUCTURES, NANOMODELLING AND NANOFABRICATION
i3N