Atomistic simulations on the mobility of di- and tri-interstitials in Si

related publications (since 2001):

Posselt, M., Gao, F., Zwicker, D.,
Atomistic study of the migration of di- and tri-interstitials in silicon,
Phys. Rev. B 71 (2005) 245202

Posselt, M., Gao, F., Zwicker, D,
Migration of di- and tri-interstitials in silicon,
Nucl. Instr. Meth. B 228 (2005) 212

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methods to determine diffusion coefficients

self-diffusion coefficient per defect D_s

sum of the squared displacements of *all* atoms vs. time

$$ssd_a(t) = \sum_{i=1}^{N} (\mathbf{r}_i(t) - \mathbf{r}_i(0))^2 = const. + 6 D_s t$$

D_s: mobility of the lattice atoms due to the presence of the defect

defect diffusivity D_d

is obtained by monitoring the trajectory of the center-of-mass of the defect using the Wigner-Seitz-cell analysis

trajectory is decomposed into n_s segments

for each segment m the squared displacement is calculated

$$sd_d(m) = (\mathbf{R}(t_m) - \mathbf{R}(t_{m-1}))^2,$$

$$t_m = t_{m-1} + \Delta t$$

$$D_d = \frac{1}{n_s} \sum_{m=1}^{n_s} \frac{sd_d(m)}{6 \Delta t}$$

(tracer) correlation factor $f = \frac{D_s}{D_d}$

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di-interstitial

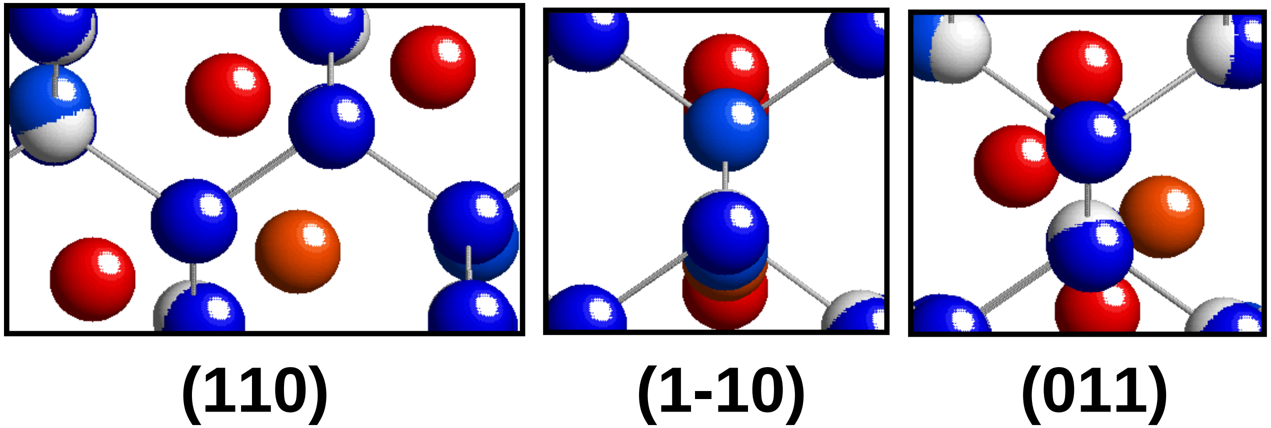
structure and energetics

I_2^A

"Z structure" (C_{2h})

E_f = 6.10 eV

E_b = 1.74eV



CP: Gilmer 1995 (SW): 5.70 eV; Marques 2001 (T3): 6.32 eV

TB: Rasband 1996: 8.0 eV; Hane 2000: 5.85 eV

DFT: *Richie 2004: 6.46 eV*

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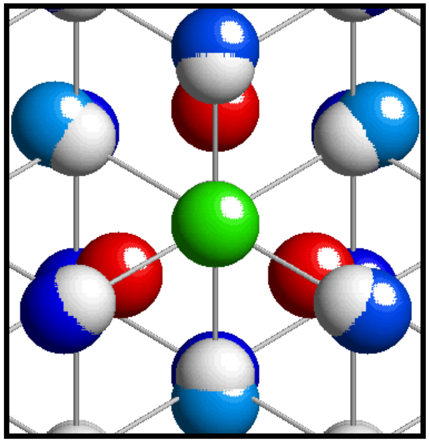
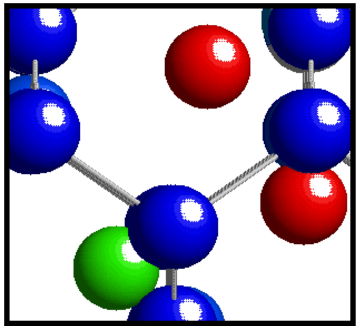
I_2^B *"modified triangle in {111}" (C_{1h})*

E_f = 6.14 eV

E_b = 1.70 eV



(111)



(1-10)

DFT: *Richie 2004: 6.46 eV*

similar configuration (found by TB and DFT): "triangle in {111}" (C_{1h})

TB: Rasband 1996: 7.3 eV; Hane 2000: 5.64 eV; Bongiorno 2000: 4.91 eV

DFT: Kim 1999: 4.9-6.0 eV; Jones 2002: 5.19 eV; Chichkine 2002: 4.84-4.96 eV;

Richie 2004: 5.66 eV; Lopez 2004: 5.76-5.84 eV

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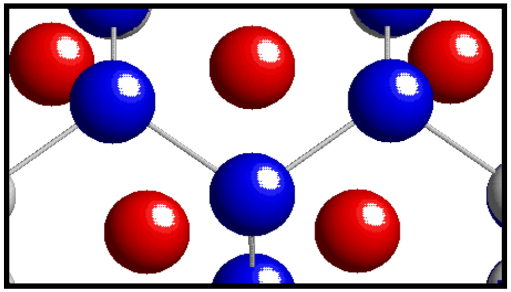
I_2^C

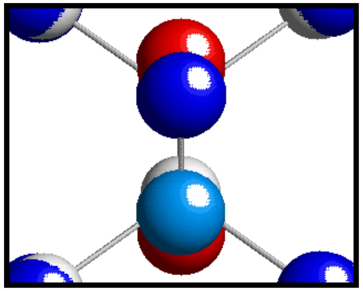
"W structure" (C_{2v})

E_f = 6.37 eV

E_b = 1.47 eV



(110)

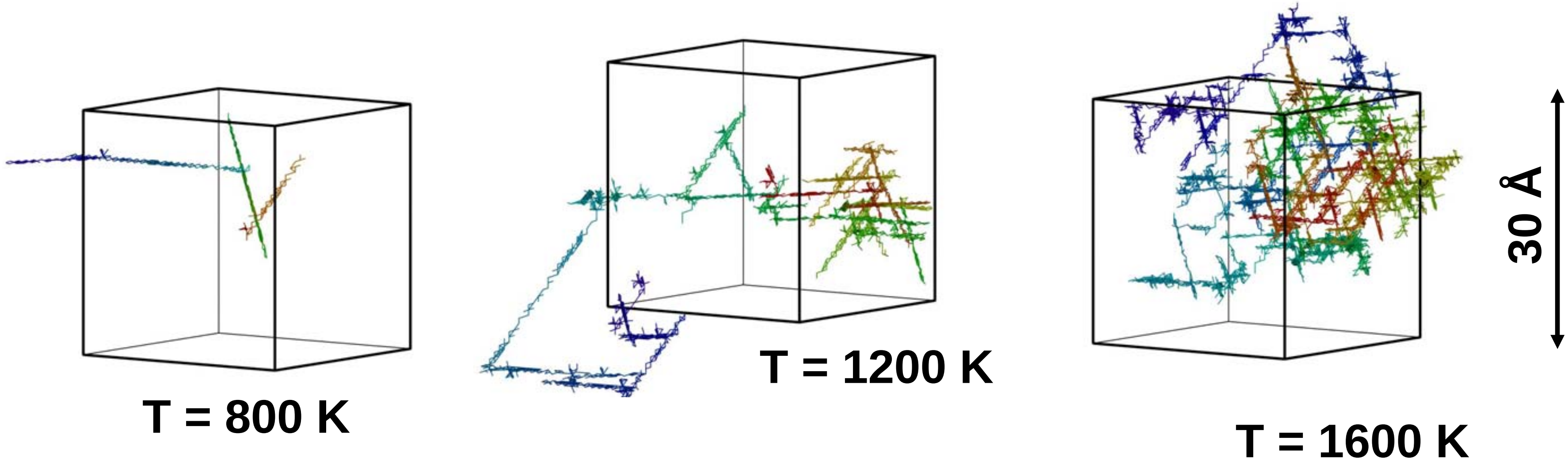


(1-10)

TB: Rasband 1996: 7.7 eV; Hane 2000: 6.07 eV

migration

center of mass trajectories over a period of 4.4 ns



temperature dependent migration mechanism

low T – high mobility along <110> axes, change between equivalent directions occurs seldom and requires a long time

high T – frequent change between equivalent <110> directions

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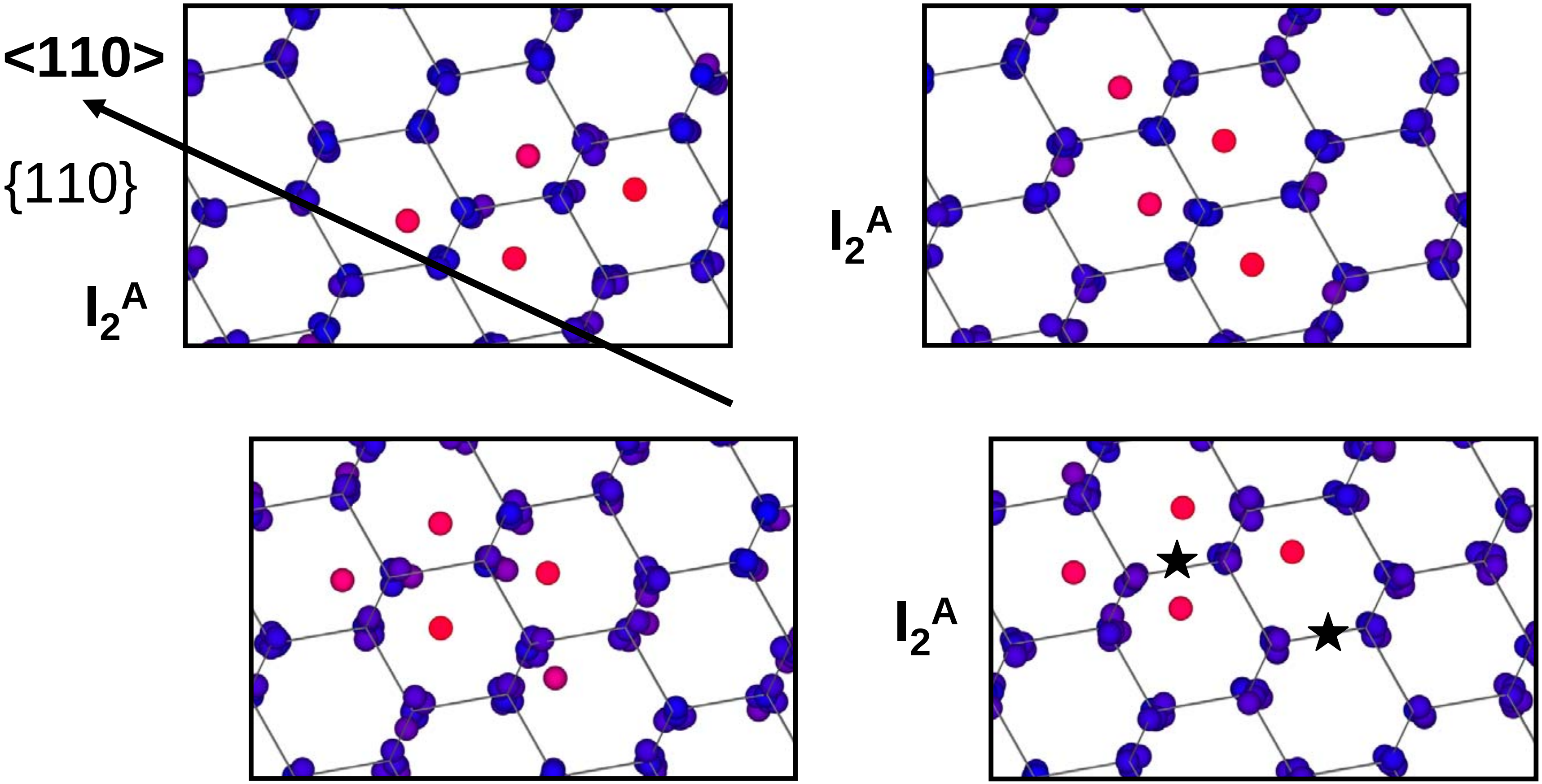
migration along <110>: in a {110} plane, as I_2^A ...

2 ps

snapshots: **migration distance: *2nd n.n. distance***



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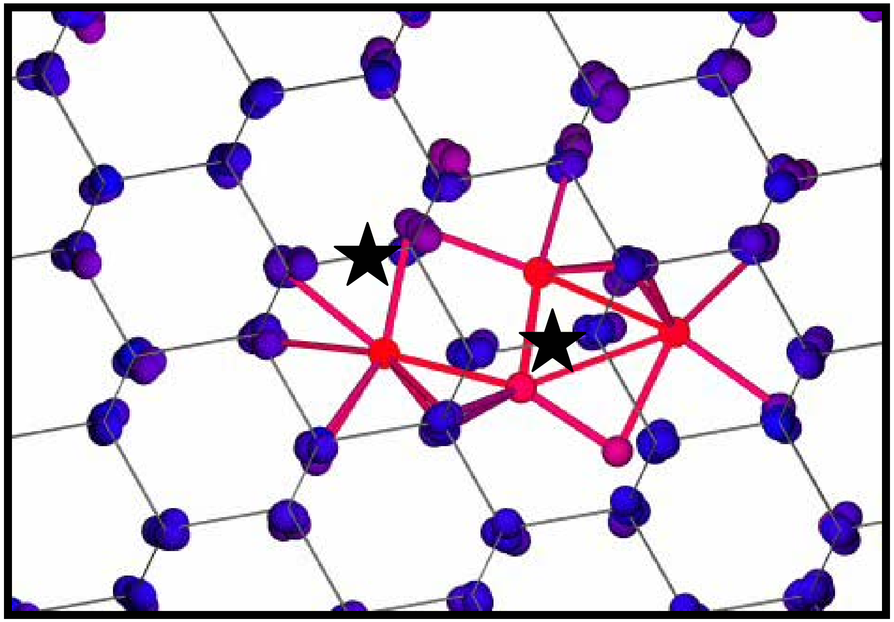
movie 1c
(~3 ps)

migration distance:
2nd n.n. distance

{110}

atoms belonging to the defect change continuously

bond switching



place the cursor on the figure and double click to start the movie

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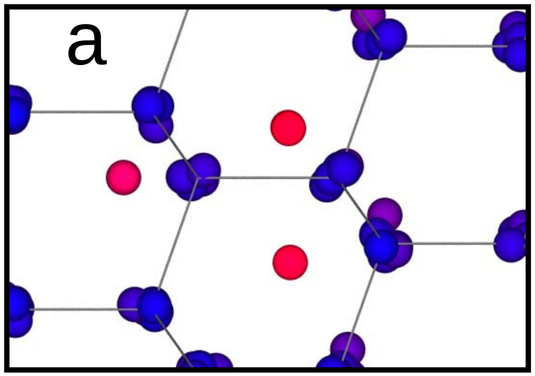
change between different <110> directions ({110} planes)
via transformation: $I_2^A \rightarrow I_2^B$ (immobile) $\rightarrow I_2^A$

1 ps

{110}

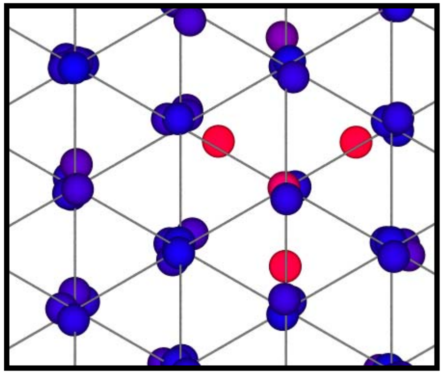
<111>



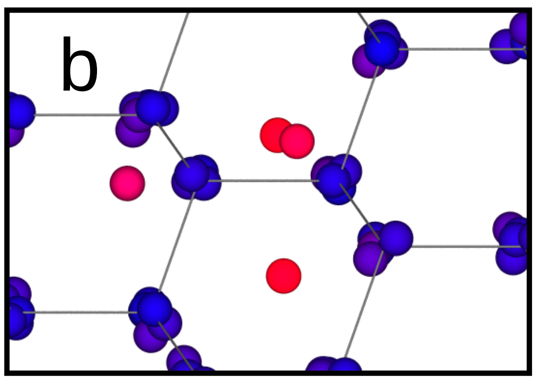
I_2^B

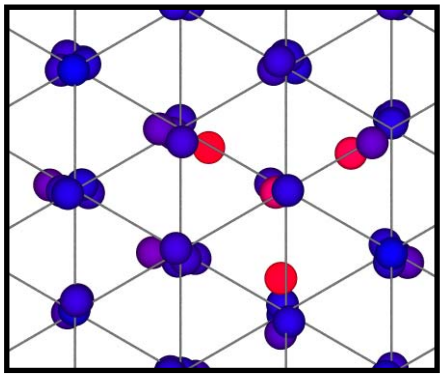
{111}

<110>



rotation out of the {111} plane





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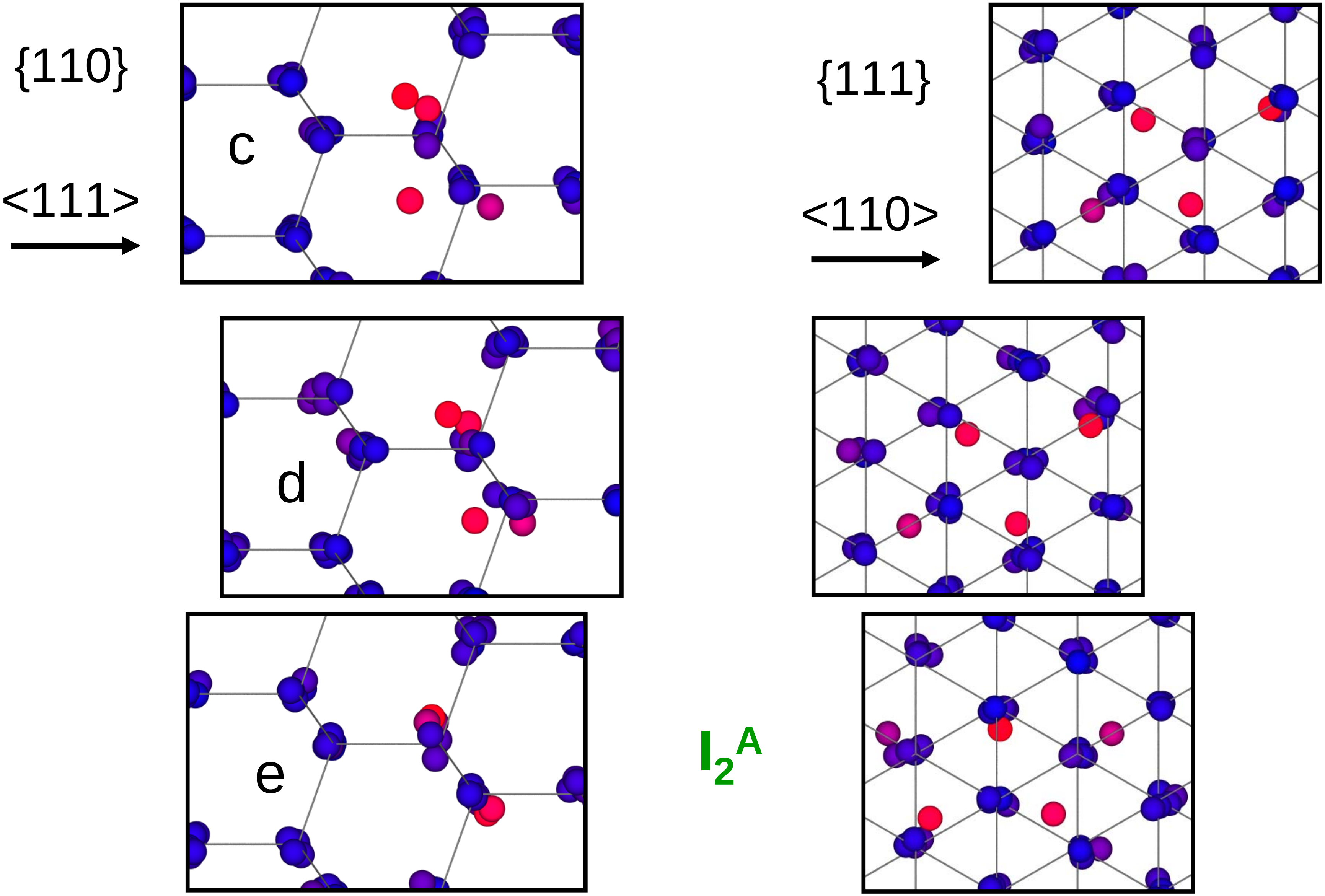

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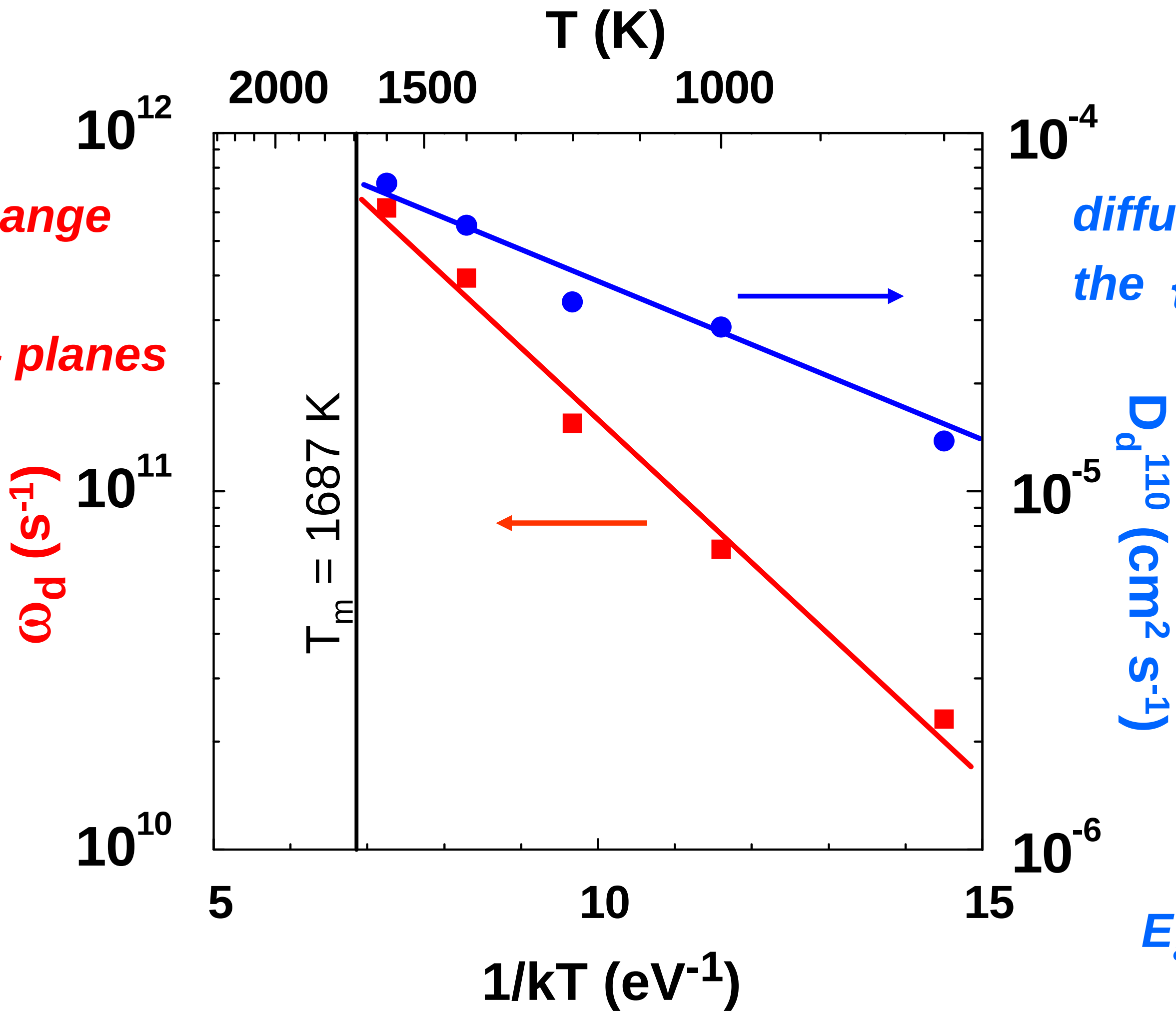
detailed analysis of migration of the di-I

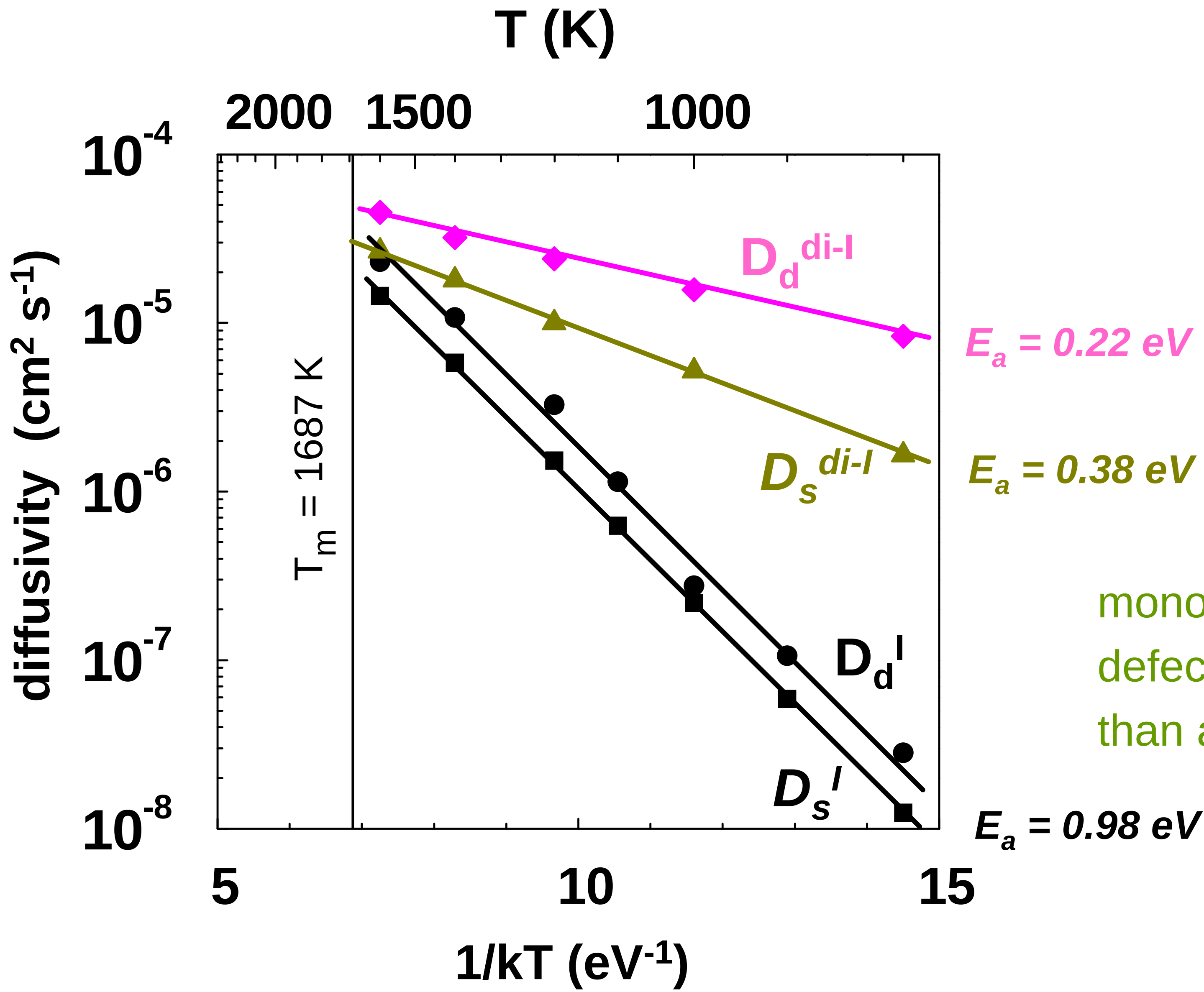


rate for the change between different {110} planes

diffusivity within the {110} planes

E_a = 0.46 eV

E_a = 0.20 eV



highly mobile

mono and di-I:
defect mobility higher than atomic mobility

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tri-interstitial

structure and energetics

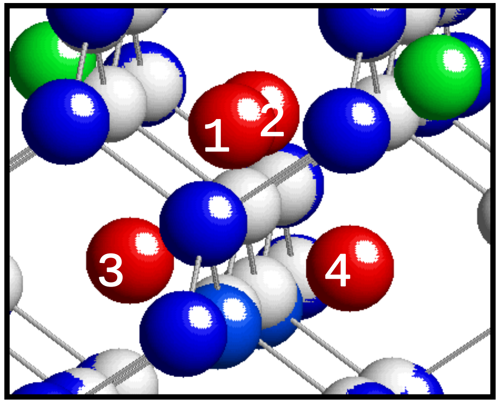
I_3^A

“mod. tetrahedron” (C_{2v})

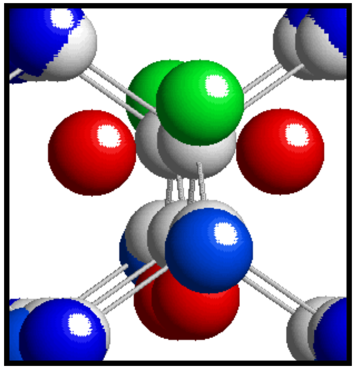
E_f = 7.54 eV

E_b = 4.22 eV

[001]



near (110)



near (1-10)

CP: Gilmer 1995 (SW): 7.08 eV; Lenosky 2000 (EDIP): 8.85 eV; Lenosky 2000 (L): 6.03 eV

similar configuration (found by TB and DFT): “tetrahedron” (C_{2v})

TB: Bongiorno 2000: 6.69 eV; Lenosky 2000: 7.83

DFT: Kim 2000: ~6 eV; Chichkine 2002: 6.05 eV;

Richie 2004: 6.96-7.11 eV; Lopez 2004: 7.27 eV

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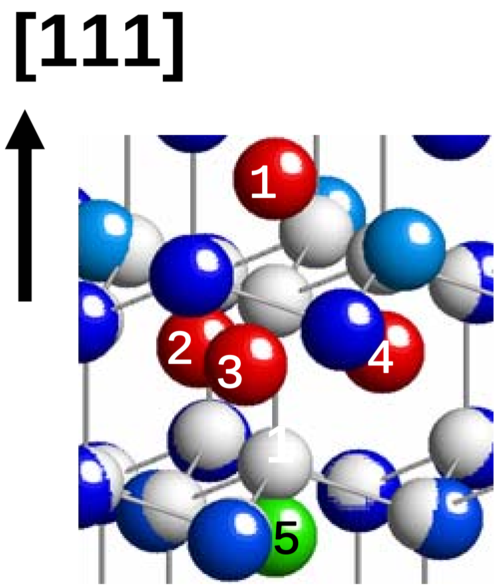
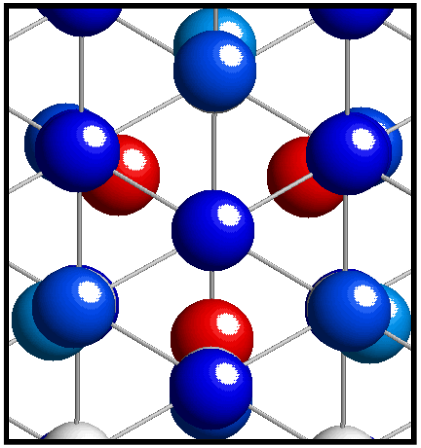
I_3^B

"mod. bond-centered triple I" (C_{3v})

E_f = 7.59 eV

E_b = 4.17 eV





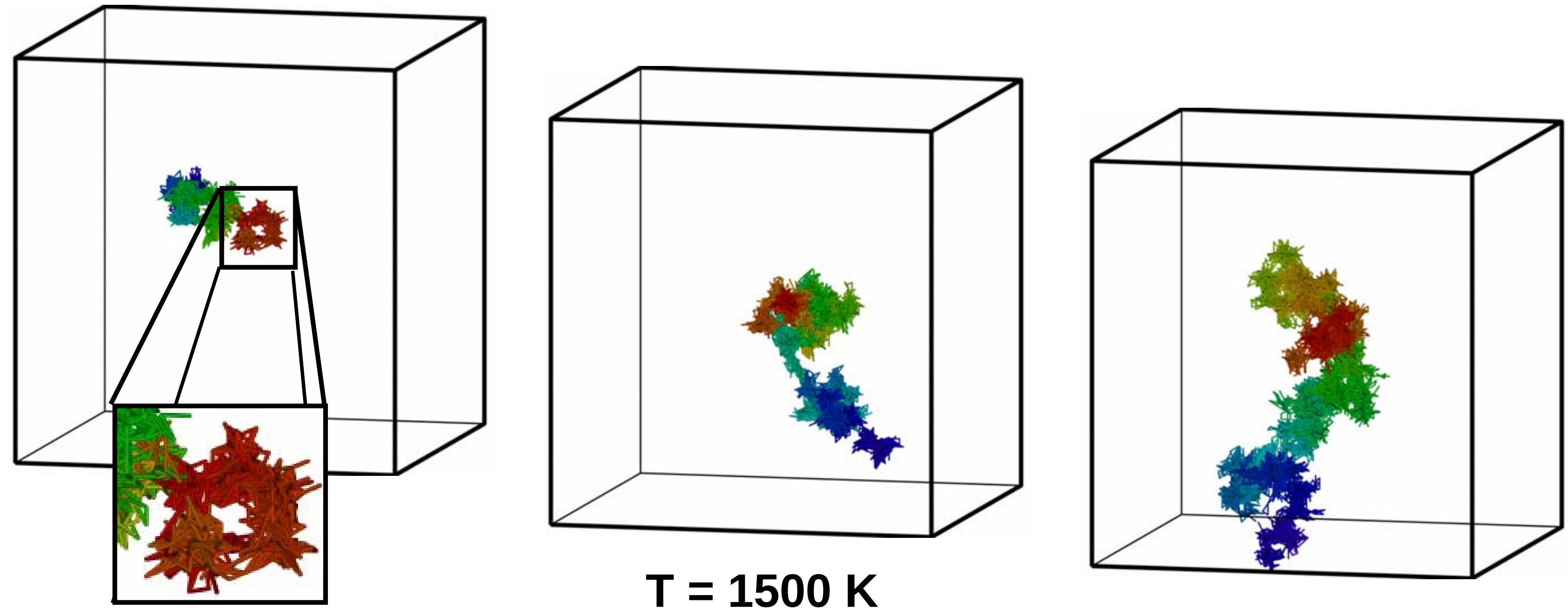
(111)

similar configuration (found by DFT): "bond-centered triple" (C_{3v})

DFT: Chichkine 2002: 6.09 eV; *Lopez 2004: 7.32 eV*

migration

trajectories over a period of 14.4 ns



T = 1500 K

T = 1600 K

T = 1400 K

complex trajectories, e.g. around a six member ring

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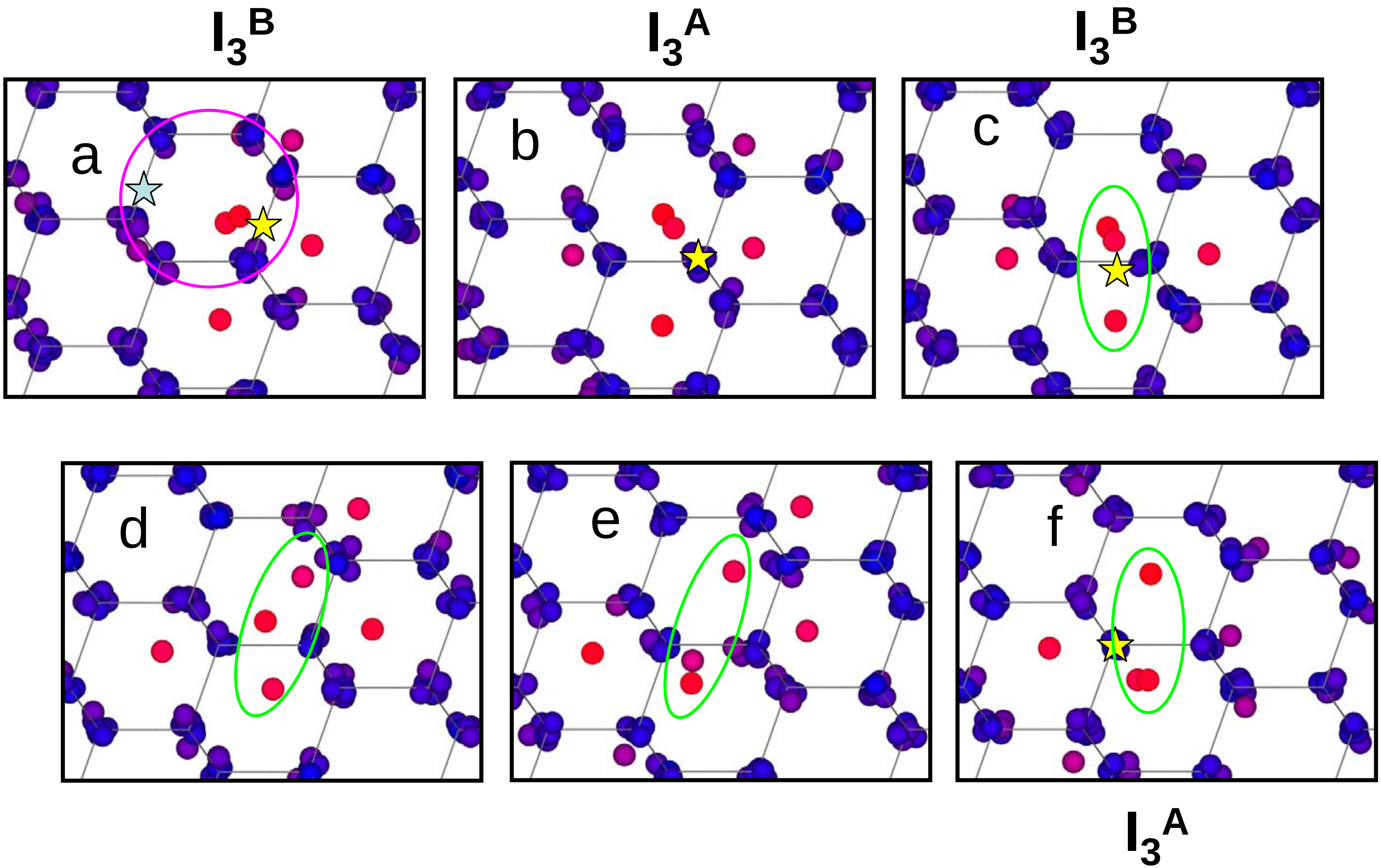
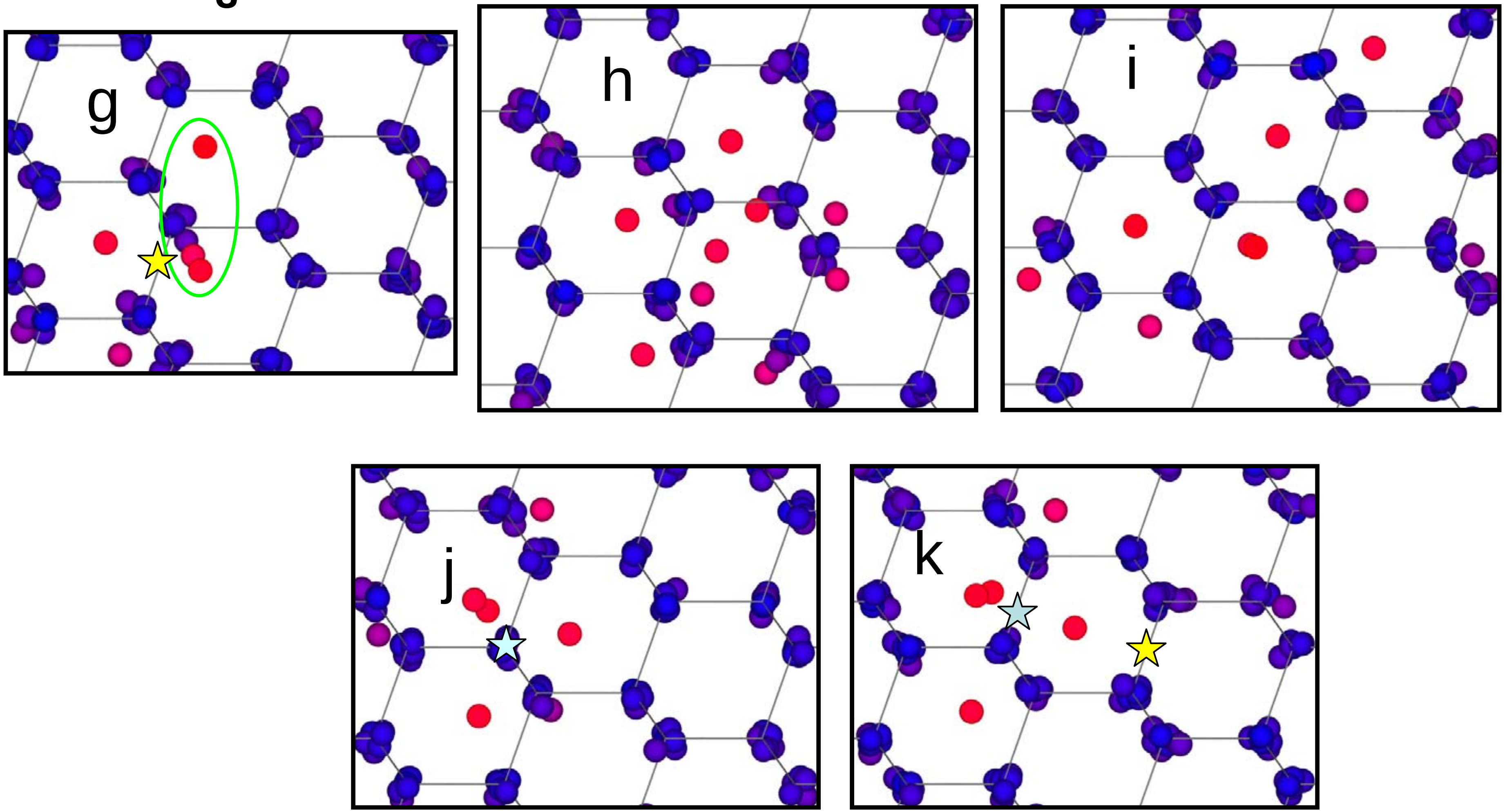
35 ps



I_3^B



I_3^A I_3^B

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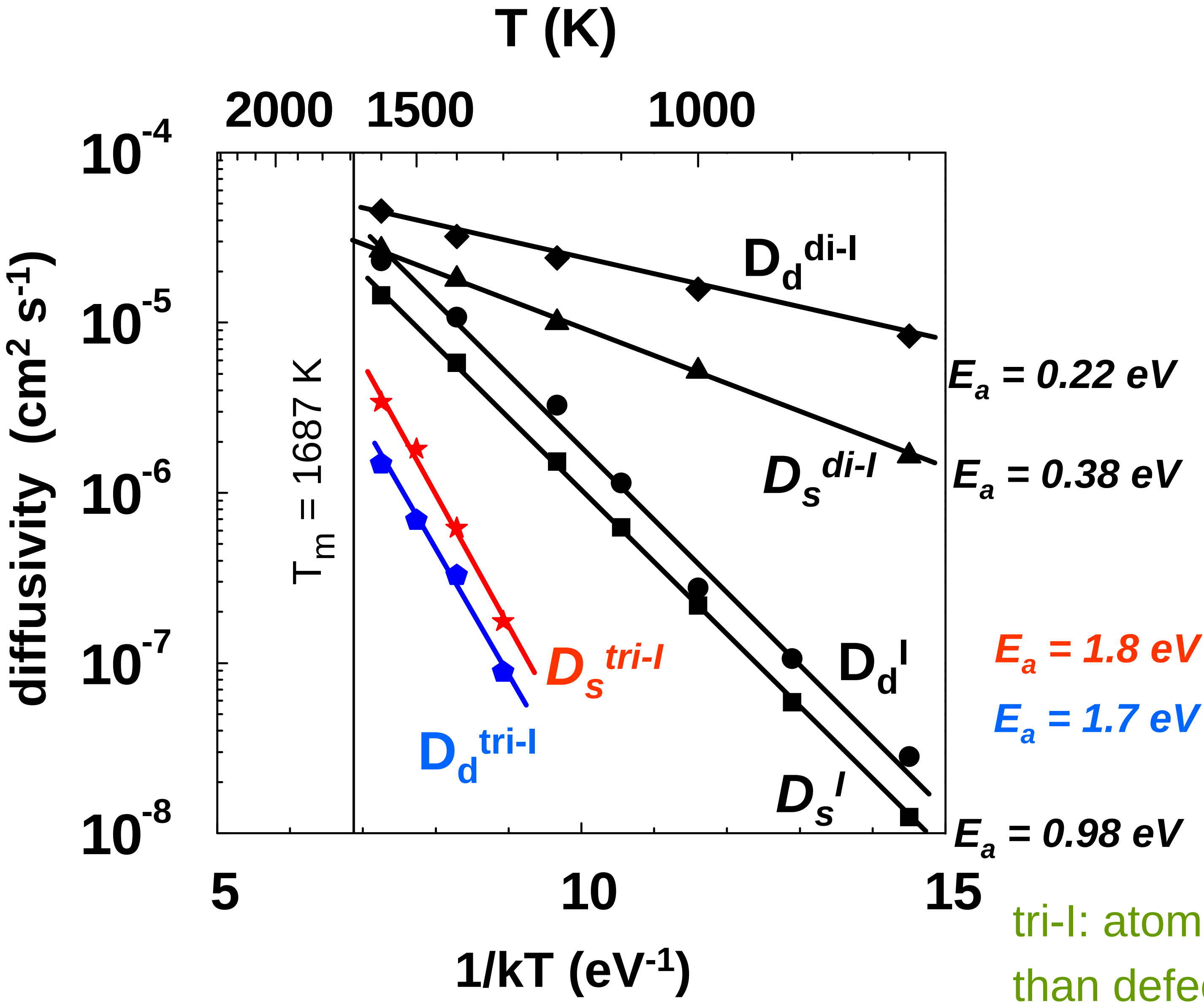

tri-I: atomic mobility higher than defect mobility

comparison with experimental data (di- and tri-I)

a) "direct" observation of di- and tri-I (?)

EPR P6 center related to di-I? pro: Lee 1976, 1998

contra: Jones 2002

PL W center related to tri-I? pro: Jones 2002

contra: Lopez 2004

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b) "indirect" proofs for the existence of di- and tri-I

state-of-the-art description of defect evolution and TED of dopants (B) during post-implantation annealing:

Cowern et al. 1999…, Pelaz et al. 1997 …

formation of interstitial clusters must be assumed

During ion implantation **only mono-interstitials and mono-vacancies** are formed. Their concentration is much higher than in the thermodynamic equilibrium.

but - atomistic simulations of defect formation reveal:
large variety of as-implanted defects is formed (also di- and tri-I)

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The **mono-interstitial and the mono-vacancy are the only mobile intrinsic defects**. They **recombine or form immobile clusters**. In particular self interstitial clusters - amongst them the di-interstitial - are introduced to obtain a transient storage of self-interstitials and to explain quantitatively the formation of {311} defects and dislocation loops as well as the TED

but - present investigations: mobile di- and tri-I

Cowern 1998...: OR model for defect evolution

start: only I +1

40 keV Si

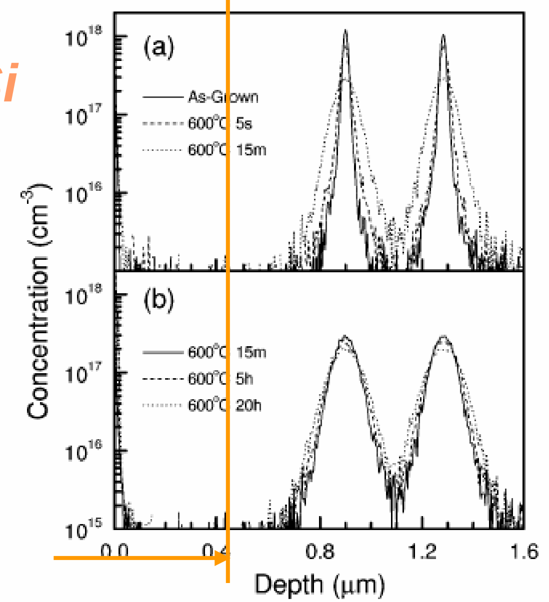


FIG. 1. B concentration profiles before and after annealing for a range of times at 600 °C.

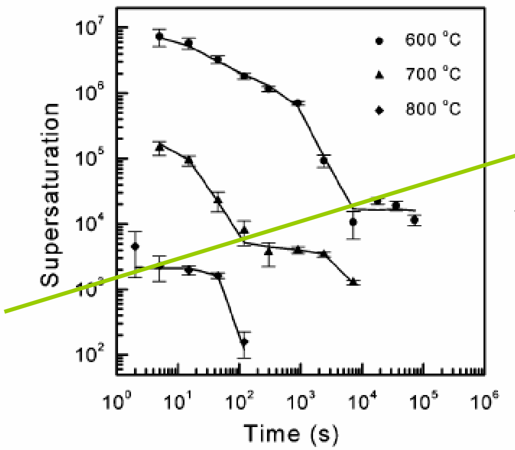


FIG. 2. Interstitial supersaturation, S, as a function of annealing temperature and time. Symbols with error bars represent experimental values with 2σ uncertainties. Curves represent fits using an Ostwald ripening model (see text).

$S = D^B/D_{eq}^B$

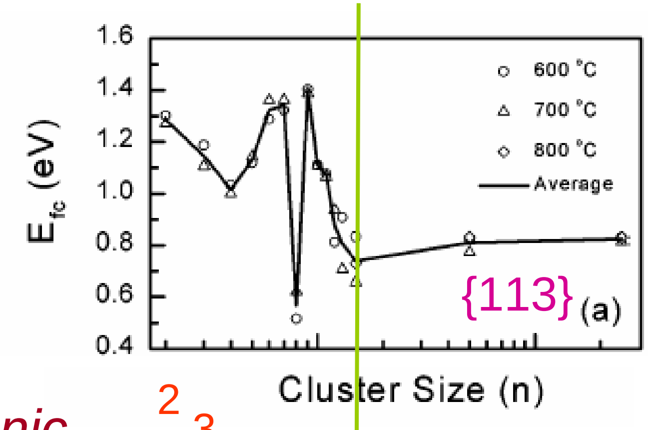
$$E_b^c = Q^I - E_m^I - E_{fc}$$

$Q^I \sim 4.5$ eV

$E_m^I \sim 1$ eV

$E_b^{di\text{-}I} \sim 2.2$ eV 1.7 eV

$E_b^{tri\text{-}I} \sim 2.3$ eV 2.5 eV



$E_b^c(n)$ non-monotonic

Forschungszentrum Dresden Rossendorf

Mitglied der Leibniz-Gemeinschaft

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Pelaz 1997...: KMC simulation of defect evolution **and** TED

start: V,I from BCA

40 keV Si

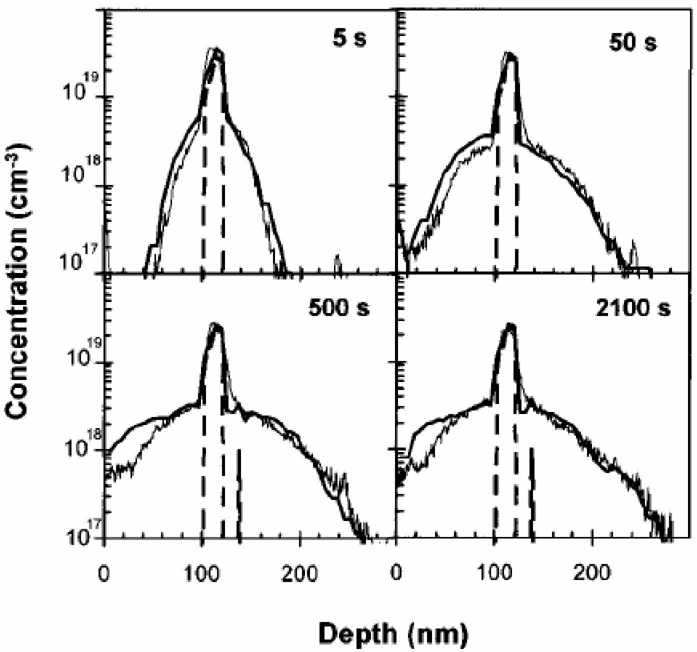

FIG. 2. Simulated and experimental profiles of a 4.5×10^{19} cm^{-3} B spike after 40 keV 9×10^{13} cm^{-2} Si implant and 5, 50, 500, and 2100 s anneal at 800 °C. Thin lines represent experimental data, thick solid lines the simu-

$E_b^{di\text{-}I}$ ~ 1.6 eV   1.7 eV

$E_b^{tri\text{-}I}$ ~ 1.8 eV   2.5 eV

$E_b^c(n)$ monotonic

Aboy 2003: $E_b^c(n)$ of Cowern
E_m^I of Bracht

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c) explanation of the long-range, trap-limited migration of implantation-induced I-like defects observed at room temperature by the high mobility of the di-I

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Kyllesbech Larsen et al. 1996:

implantation and ex-situ SRP measurements of deactivation

40 keV Si

$5x10^{13}$ cm^{-2}

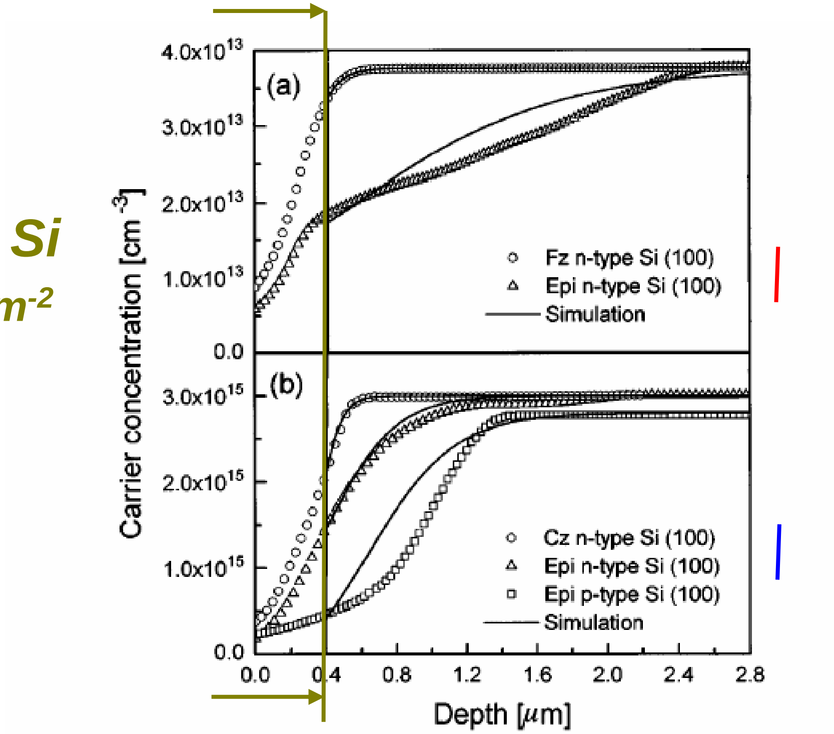

FIG. 1. SRP profiles of different homogeneously doped Si(100) substrates implanted with 40 keV ^{28}Si 5×10^{13} cm^{-2}: (a) epitaxial (Δ) and Fz (○) silicon P doped at a level of 3.7×10^{13} cm^{-3}; and (b) epitaxial (Δ), Cz (○) silicon P doped at 3.0×10^{15} cm^{-3}, and B-doped epitaxial Si (□) with a doping level of 2.8×10^{15} cm^{-3}. The solid lines are obtained

injection and trapping of I-like defects

traps:

epi: [O]<10^{15} cm^{-3}; [C]<10^{15} cm^{-3}

FZ: [O]~10^{16} cm^{-3}; [C]~10^{17} cm^{-3}

Cz: [O]~10^{18} cm^{-3}; [C]~10^{17} cm^{-3}

dopants → deactivation

a ***very low*** **fraction (~10^{-5})** of the ballistically formed defects is mobile and responsible for the deactivation

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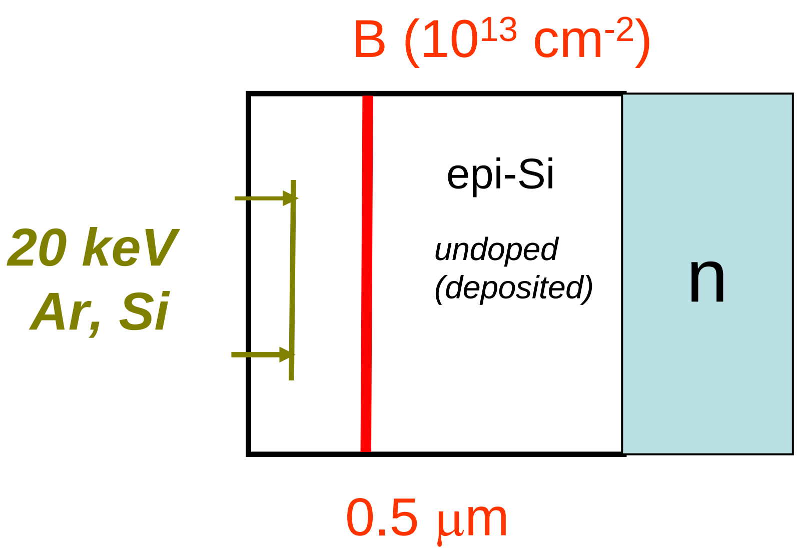
Collart 1998: *implantation and in-situ resistivity measurement*



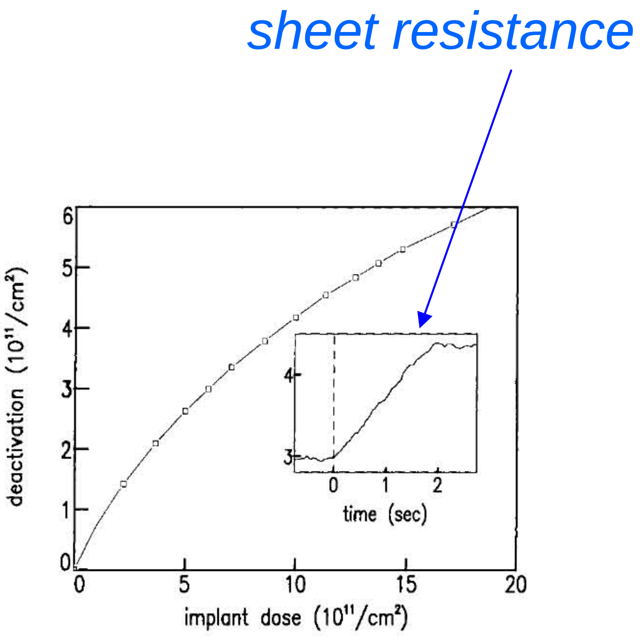


Fig. 5. Deactivation of a buried B layer as a function of Ar implant dose. The inset shows the deactivation in real time, during a two-second exposure of a previously unirradiated sample.

mobile I-like defects are formed *<u>during</u>* implantation

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Privitera 1996: *implantation and ex-situ SRP measurements*

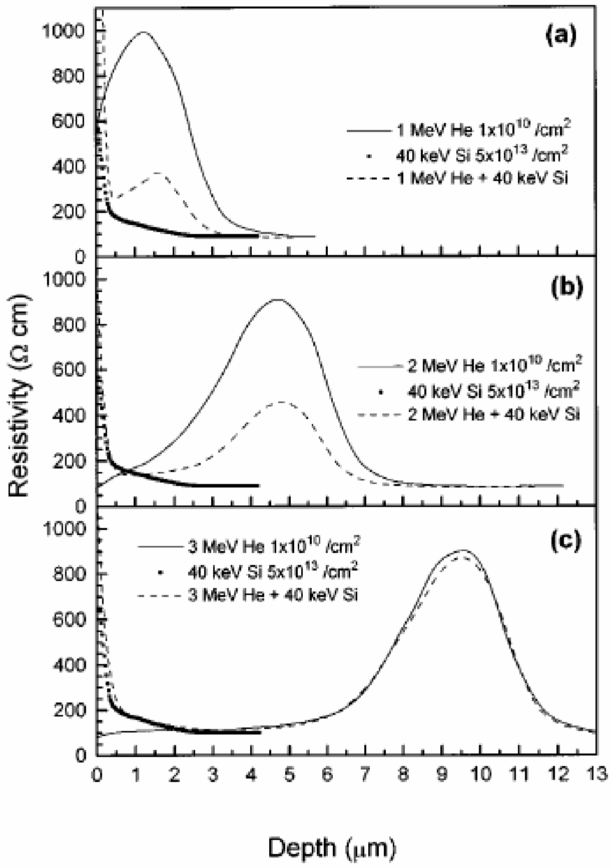

FIG. 1. Resistivity profiles for samples implanted with $1\times10^{10}/cm^2$ He (solid line), $5\times10^{13}/cm^2$ 40 keV Si (dotted line) and with both He and Si (dashed line). The energy of the He implant was 1 MeV (a), 2 MeV (b), or 3 MeV (c).

epi: [O]<10^{16} cm^{-3}; [C]<10^{16} cm^{-3}

n (phosphorus) doped ~10^{14} cm^{-3}

Si implants: deactivation by I-like defects

He implants: deactivation by V-like defects

Si after He:

reduction of deactivation by V-like defects

due to injection and trapping of I-like defects

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lower bounds of the diffusivity of the I-like defects:

10^{-11} cm^2 s^{-1} (Kyllesbech Larsen, Privitera),

10^{-7} cm^2 s^{-1} (Collart)

if this were the value for the mono-I diffusivity at RT:

- about twenty orders of magnitude larger than D^I(RT) obtained by diffusion experiments near the thermodynamic equilibrium (Bracht 1998…).
- much (5-10 orders of magnitude) larger than the mono-interstitial diffusivity often used in the interpretation of defect evolution and transition-enhanced diffusion of boron during post-implantation annealing (Pelaz 1997…)
- larger than many theoretical results (Colombo 2002)

it could be the value for the di-I diffusivity (10^{-8} cm^2 s^{-1})!

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