Interstitial contribution to self-diffusion in Si: Dependence of the correlation factor on the migration mechanism

related publication:

M. Posselt, F. Gao, H. Bracht:
Correlation between self-diffusion in Si and the migration mechanisms of vacancies and self-interstitials: An atomistic study
Phys. Rev. B 78 (2008) 035208

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Motivation

self-diffusion via mobile V and I:

$$D_{sd} = f_V D_V C_V + f_I D_I C_I$$

correlation factors f_V and f_I:

relation between the mobility of defects and atoms

Compaan and Haven 1956/1958 *(statistical theory of diffusion)*:

diamond lattice: $f_V = 0.5$, $f_I = 0.73$

used so far in almost all papers on self-diffusion in Si

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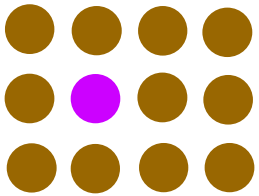
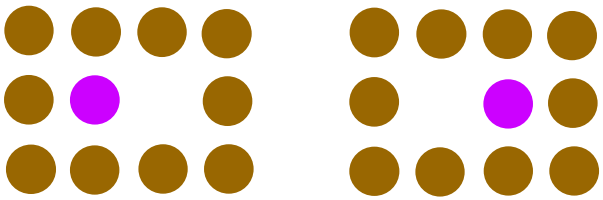
assumptions

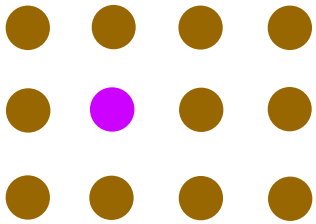
contribution of mobile V:



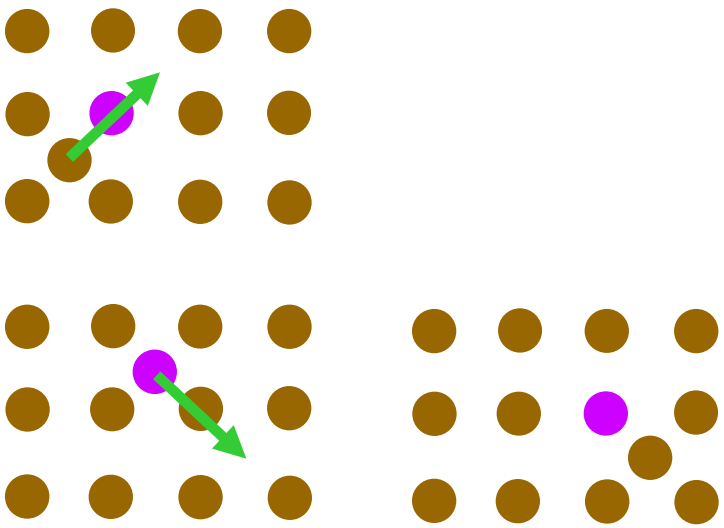
vacancy mechanism



contribution of mobile I:



interstitialcy mechanism



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Are the values of Compaan and Haven for f_V and f_I really correct?

V. Voronkov 2005

intrinsic point defects in silicon: a unified view from crystal growth, wafer processing and metal diffusion

H. Bracht 2005

simultaneous modeling of dopant (B, P, As) and self-atom diffusion

best interpretation of recent experimental data

by state-of-the-art modeling by assuming

$f_V = 0.5$ $\boxed{f_I = 0.5 - 0.6}$

this work:

determination of f_I by MD without any assumptions about the migration mechanisms

dependence on interatomic potential

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Simulation Method

two interatomic potentials: **Stillinger-Weber and Tersoff 3**

dynamic simulation of I migration: **5 – 500 ns** *(dependent on T)*

diffusivity D_I

obtained by monitoring the trajectory of the center-of-mass of the I

trajectory is decomposed into n_s segments, for each segment m the squared displacement sd(m) is calculated

$$sd(m) = (\mathbf{R}(t_m) - \mathbf{R}(t_{m-1}))^2 \qquad D_I = \frac{1}{n_s}\sum_{m=1}^{n_s}\frac{sd(m)}{6\Delta t}$$

self-diffusion coefficient D_s

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

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

D_s: mobility of the lattice atoms due to the presence of a single I

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$$D_{sd} = f_V D_V C_V + f_I D_I C_I$$

$$C_V = 0: \quad D_{sd} = f_I D_I C_I$$

self-diffusion coefficient per I:

$$D_s = \frac{D_{sd}}{C_I} = f_I D_I$$

correlation factor:

$$f_I = \frac{D_s}{D_I}$$

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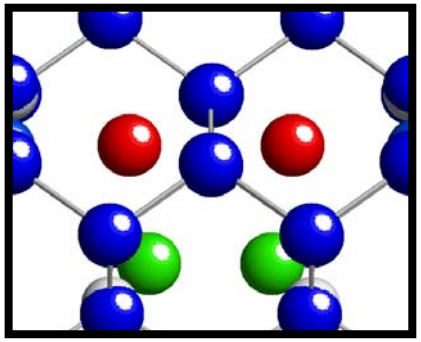
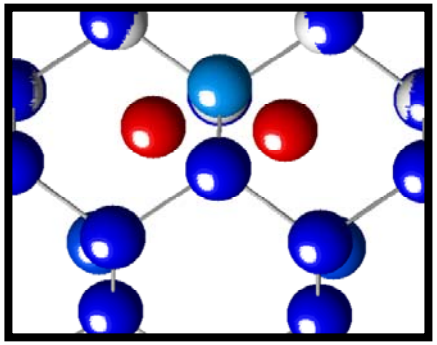
Results

I migration – SW potential



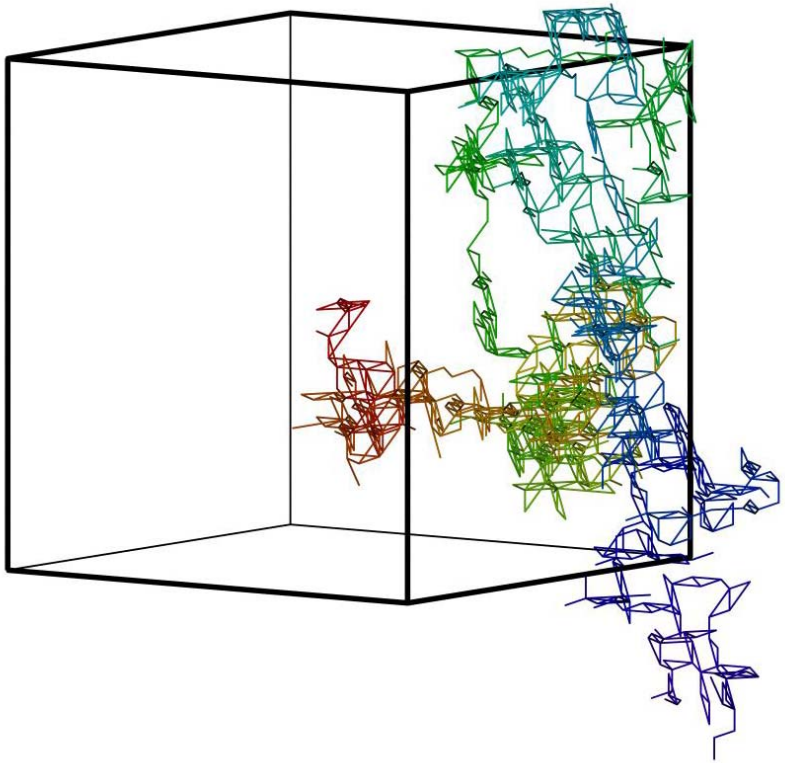
extended

<110> dumbbell



<110> dumbbell

trajectory (1600 K, 4.4 ns)



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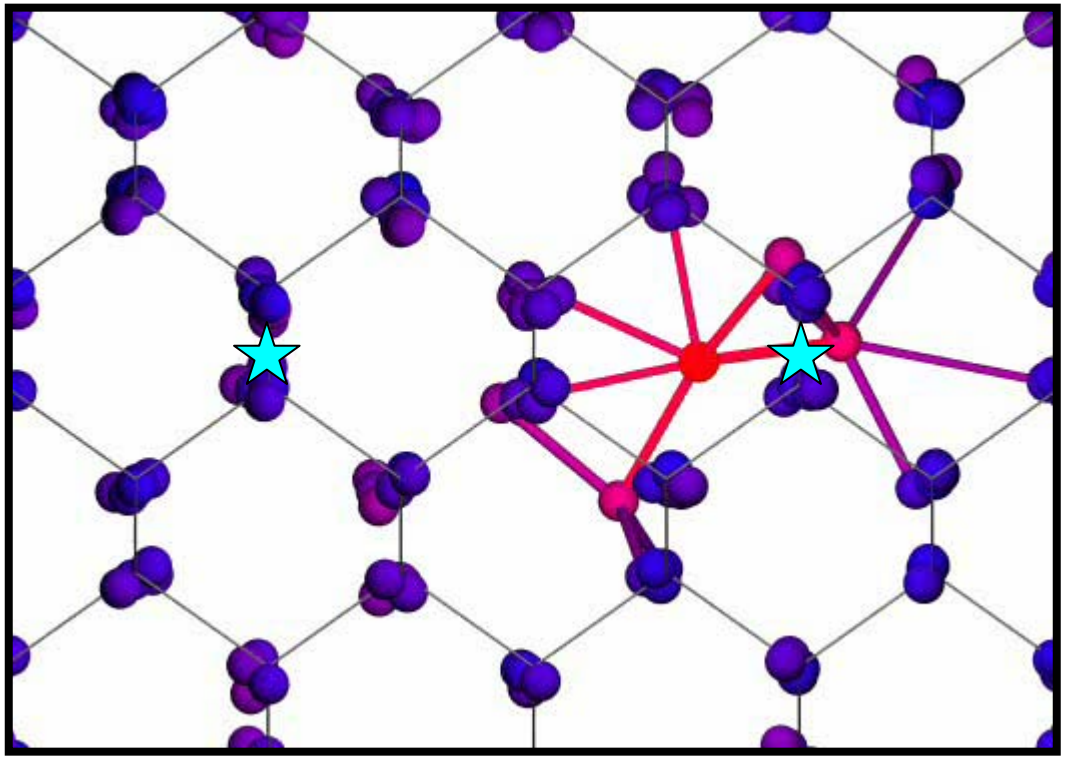
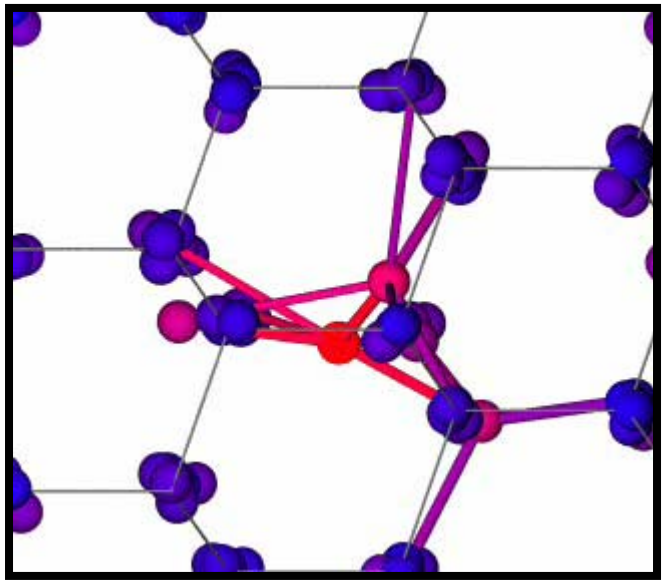
migration path I: *motion in a {110} plane – translational jump*

<110>dumbbell - <110>extended dumbbell - <110>dumbbell





(110)

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

(-110)

movie 2a

1600 K

movie 2b

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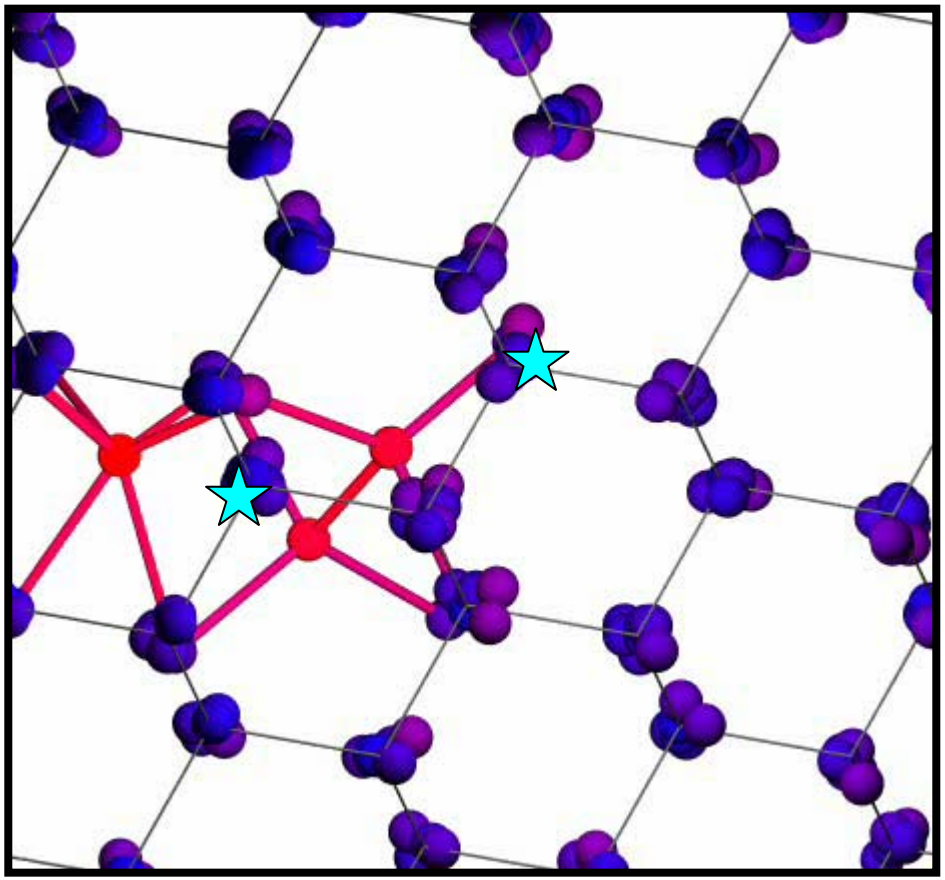
migration path II: *change between {110} planes – rotational jump*

<110>extended dumbbell -<110>dumbbell -<110>extended dumbbell

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



movie 3

1600 K

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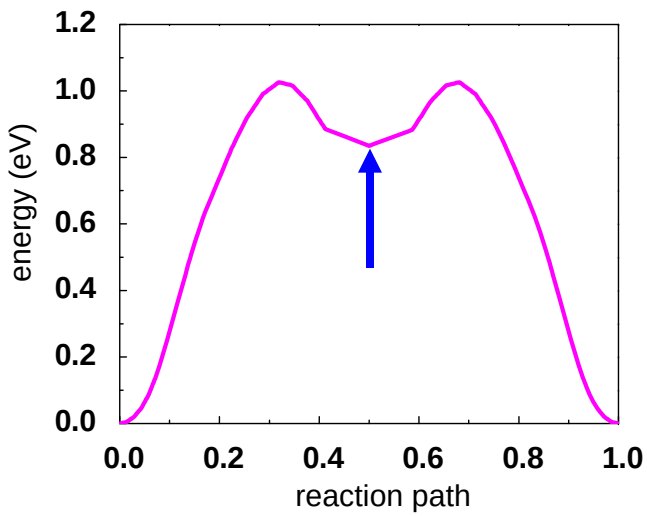
static migration barriers

migration path I

E_b = 1.03 eV (NEB)



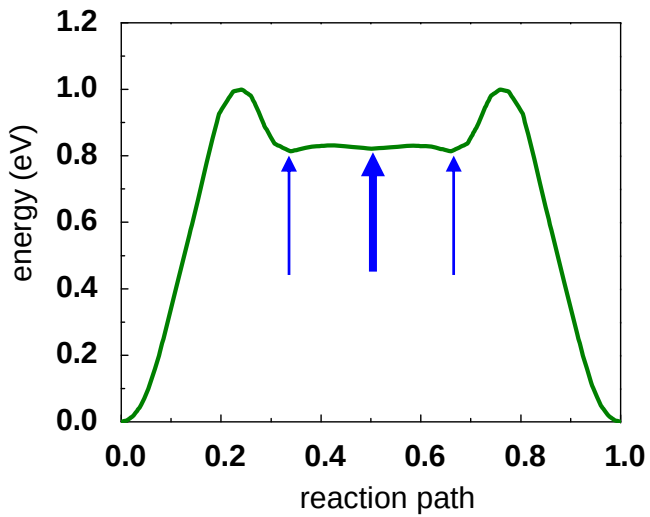
extended <110> dumbell

<110> dumbell

extended <110> dumbell

migration path II

E_a = 1.00 eV (NEB)



dynamic migration barriers and diffusivities

defect mobility higher than atomic mobility

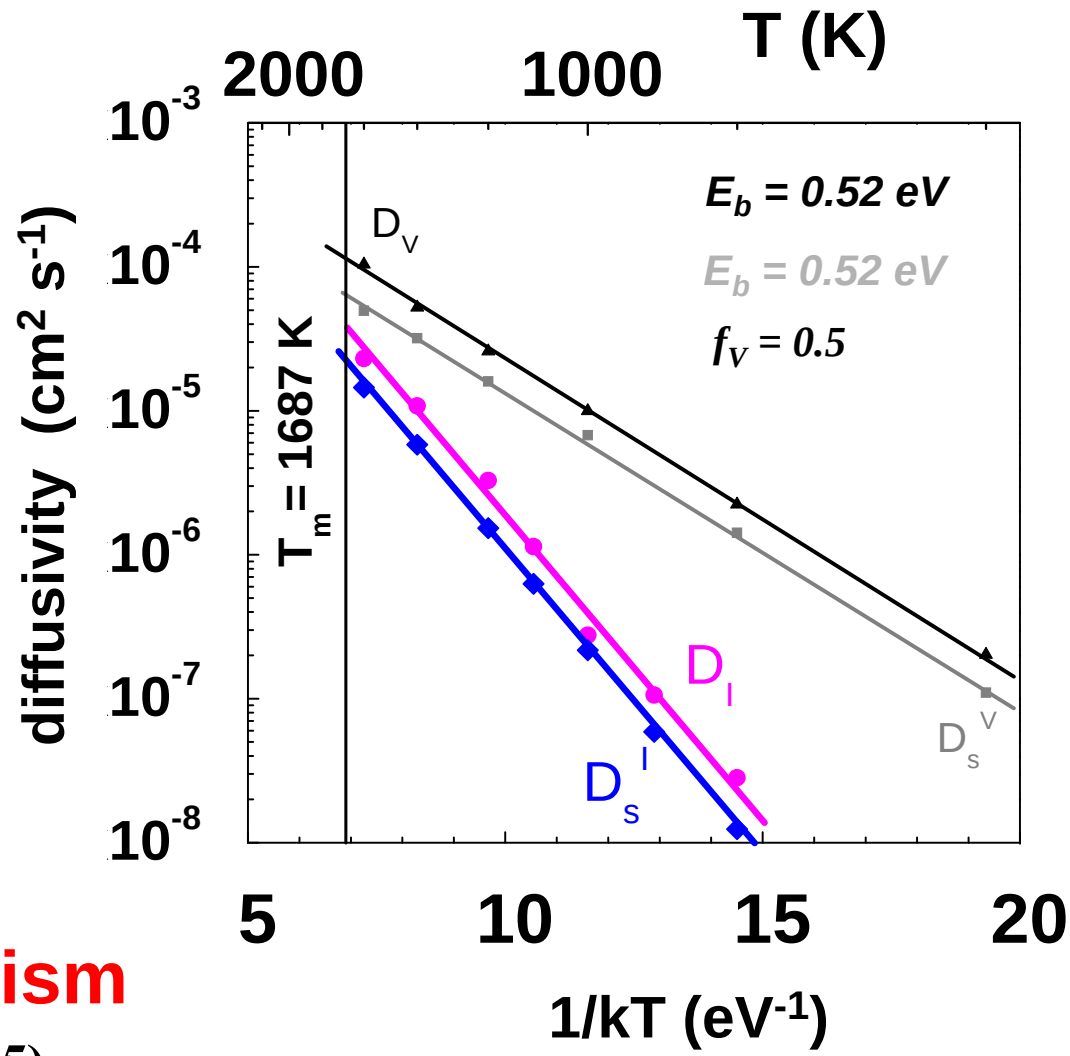
E_b = 0.98 eV

E_b = 0.98 eV

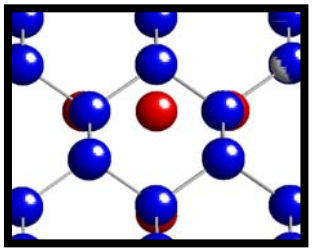
$f_I = 0.54 \ (\neq 0.73)$

dumbbell mechanism

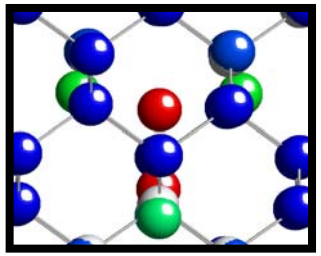
(cf. Voronkov, Bracht 2005)



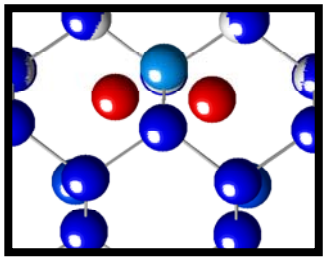
I migration – T3 potential



T

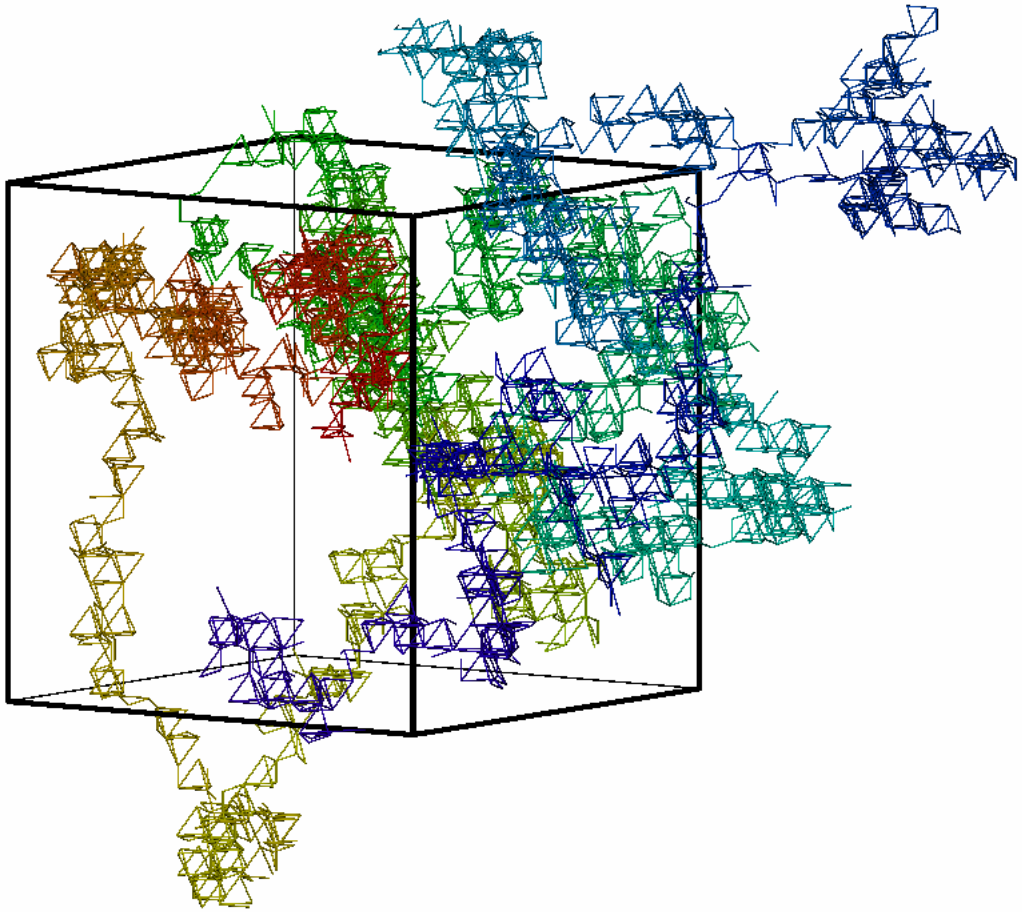


<100> dumbbell



<110> dumbbell

trajectory (1600 K, 4.4 ns)



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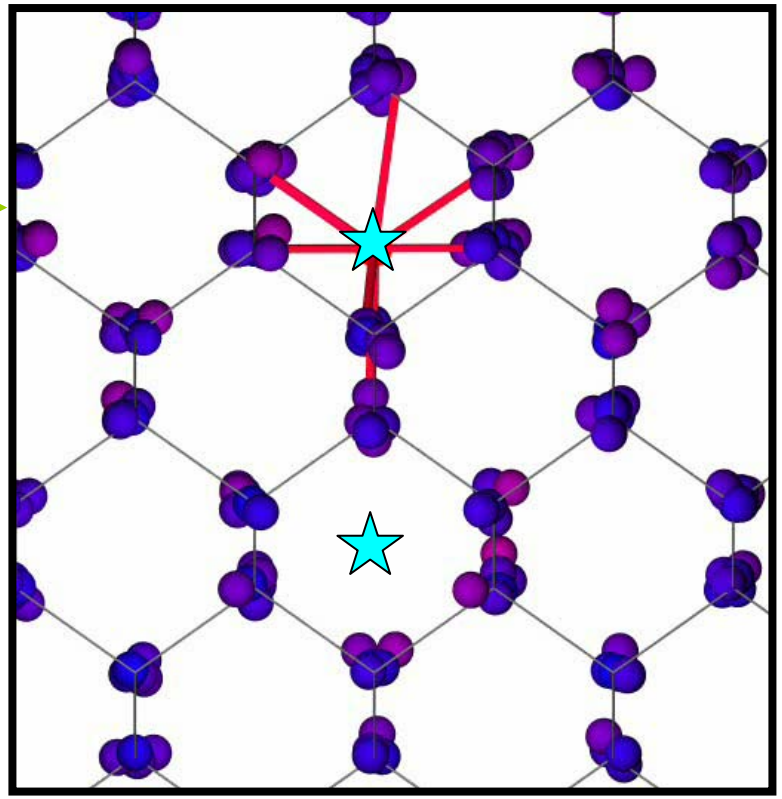
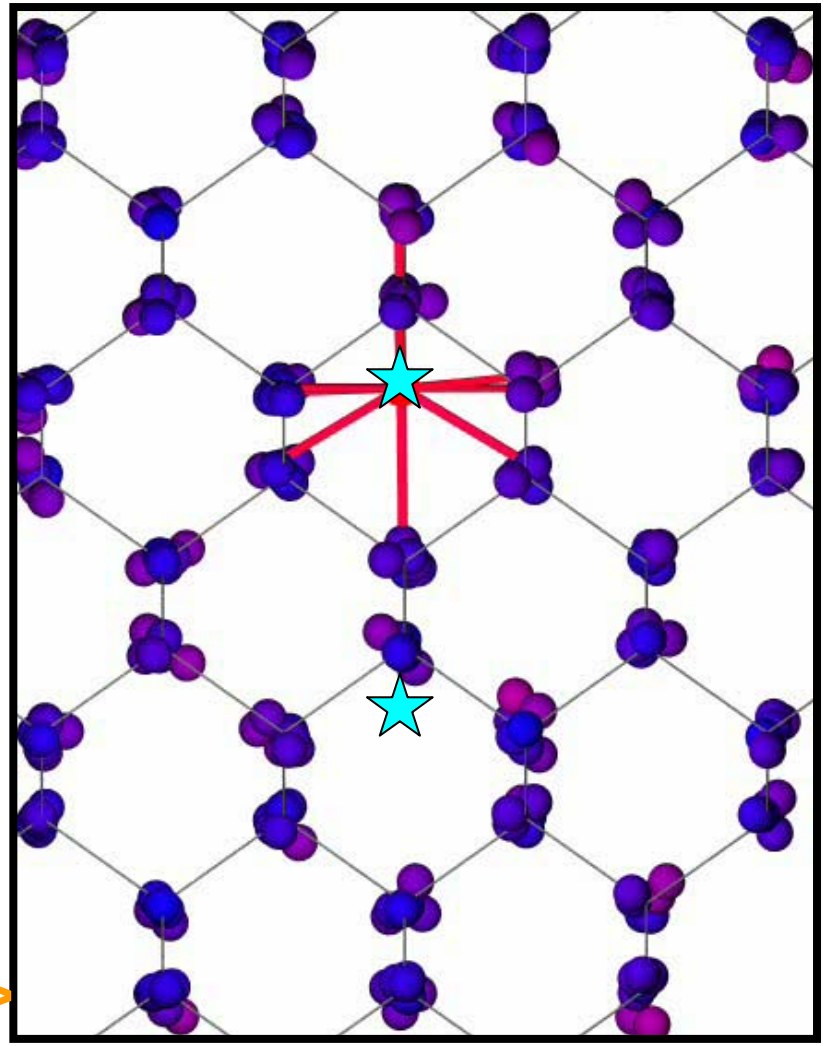
migration path I: *motion in a <100> direction*

T - <100>dumbbell - T



(110)

<100>



(-110)

movie 4a

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

1600 K

movie 4b

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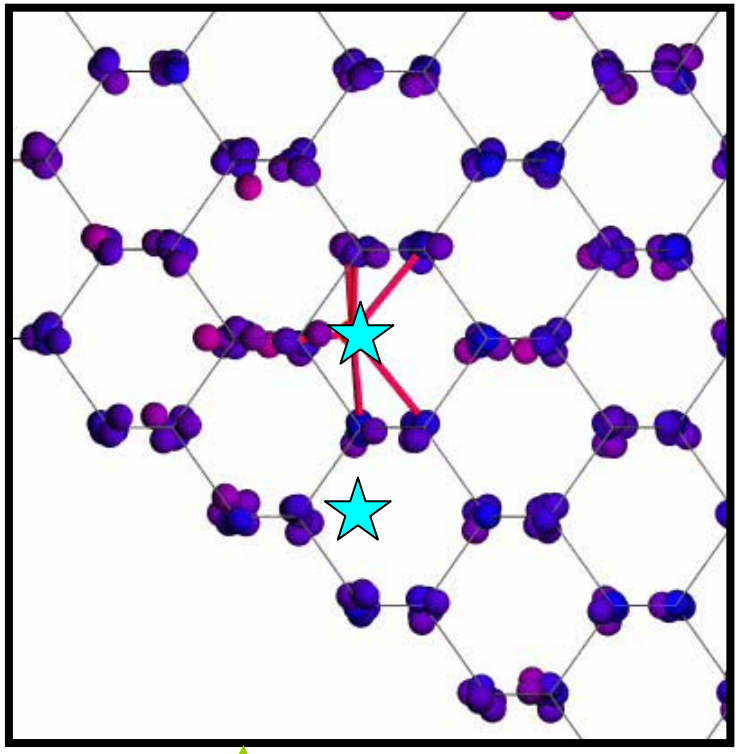
migration path II: *motion in a {100} plane*

T - <110>dumbbell - T



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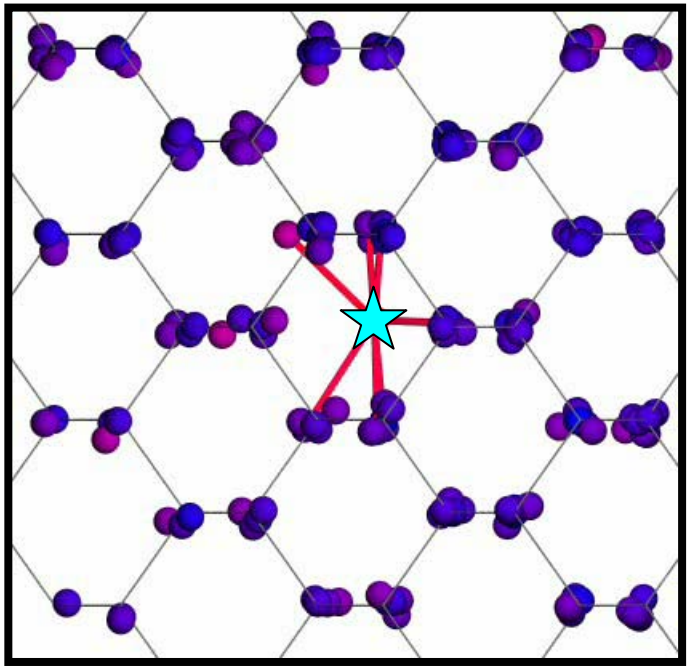

(-110)

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

movie 5a

1600 K

movie 5b

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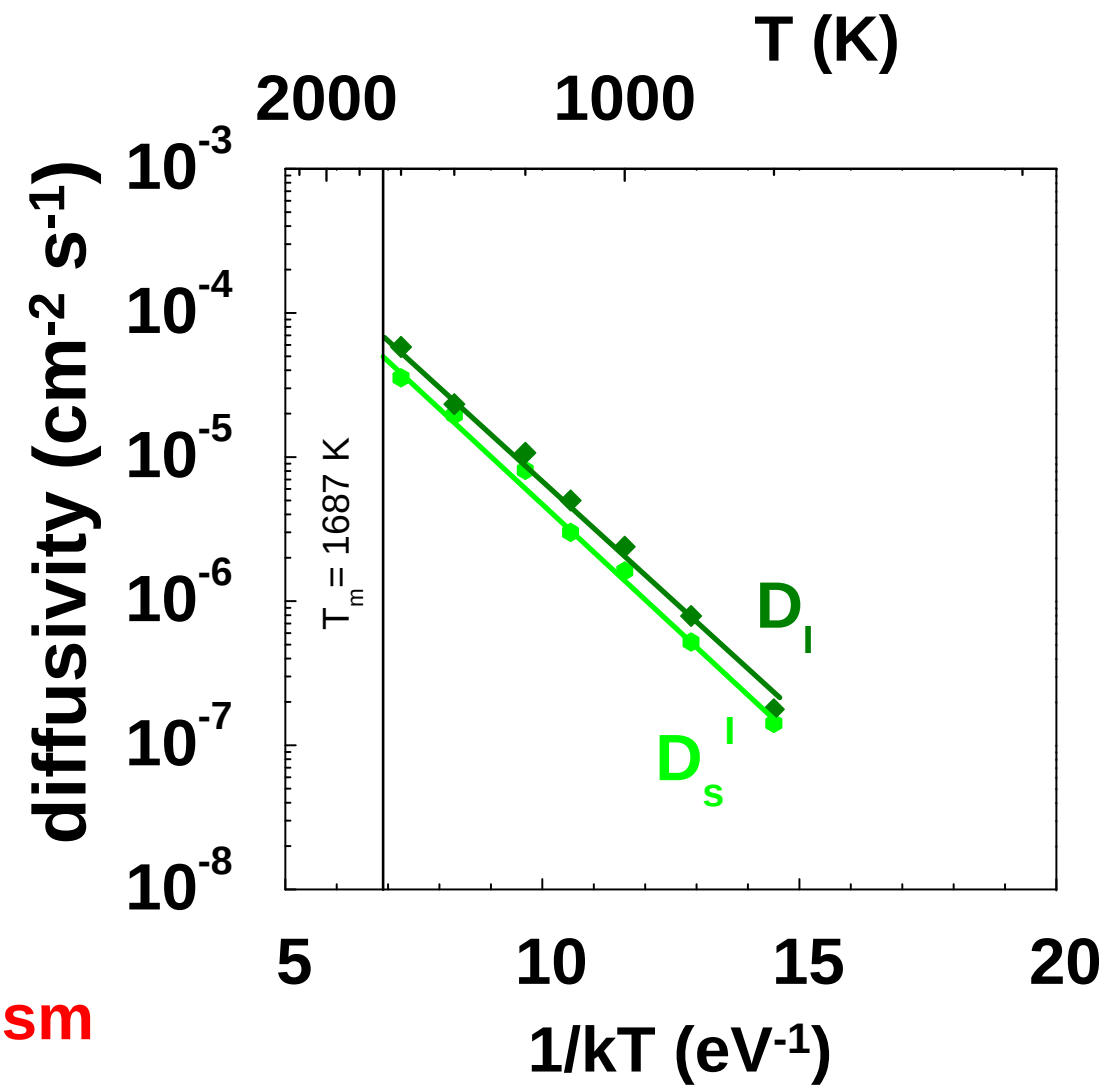
dynamic migration barriers and diffusivities



defect mobility higher than atomic mobility

$E_b = 0.75$ eV

$E_b = 0.75$ eV

$f_I = 0.71$ (~ 0.73)

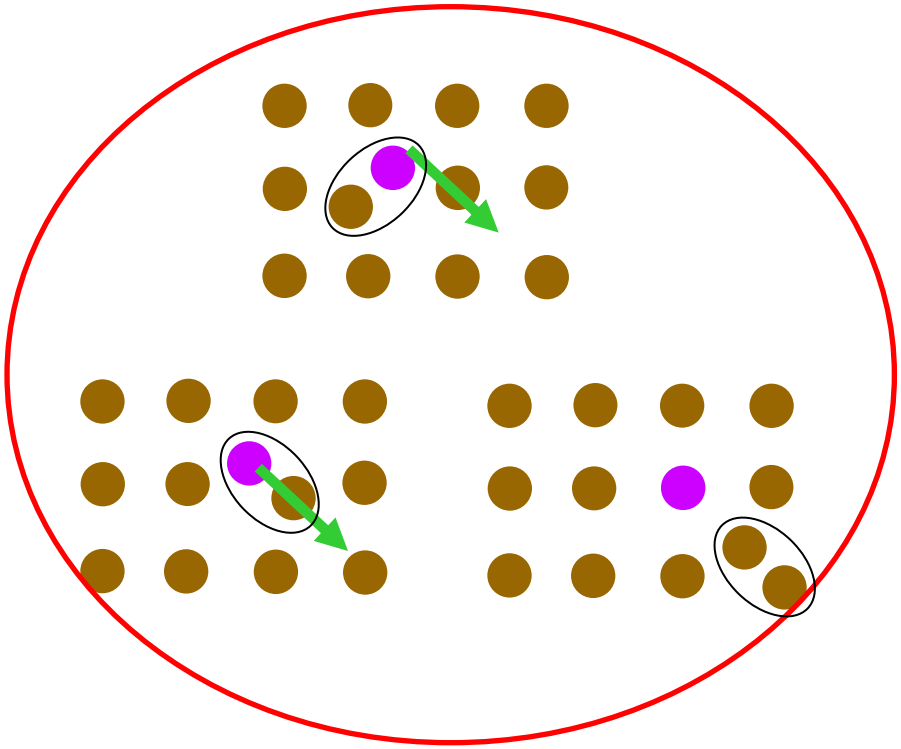
interstitialcy mechanism

(cf. Compaan and Haven)

Summary

SW

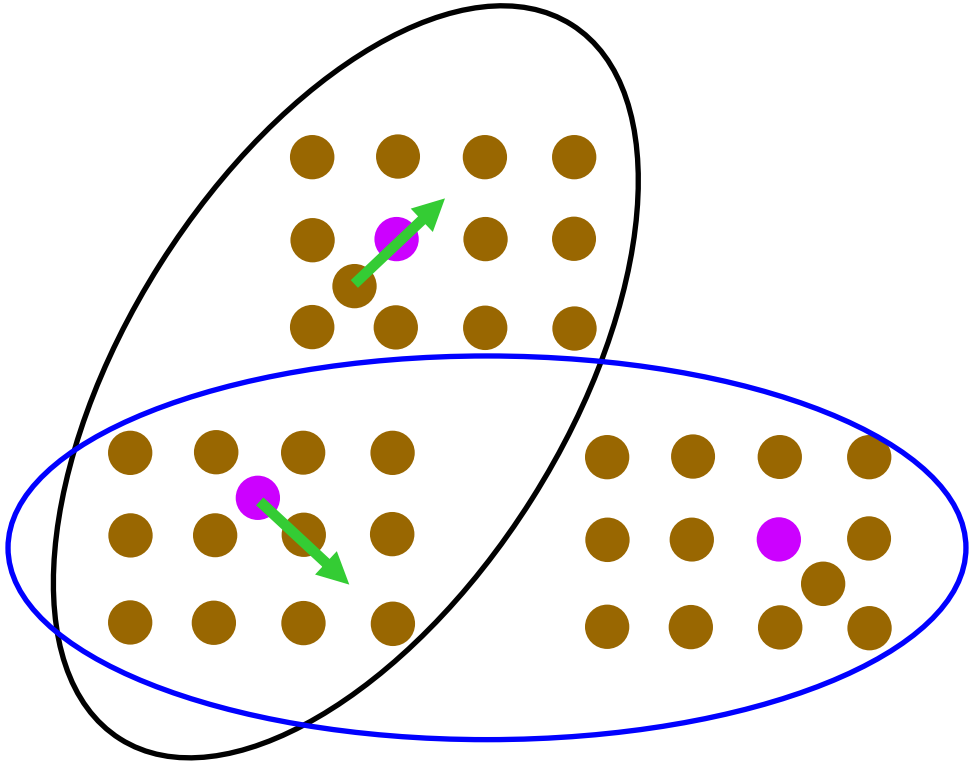
dumbbell mechanism



correlation

T 3

interstitialcy mechanism



no correlation

correlation

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MD simulations with the SW potential yield a correlation factor f_I in agreement with the analysis of recent experimental data on defect, dopant and self-atom diffusion

present results on the migration mechanisms should be independent of the absolute value of the self-interstitial diffusivity determined by the MD simulations

self-interstitial diffusion in Si occurs via the dumbbell mechanism

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