Atomistic modeling of defect diffusion in SiGe

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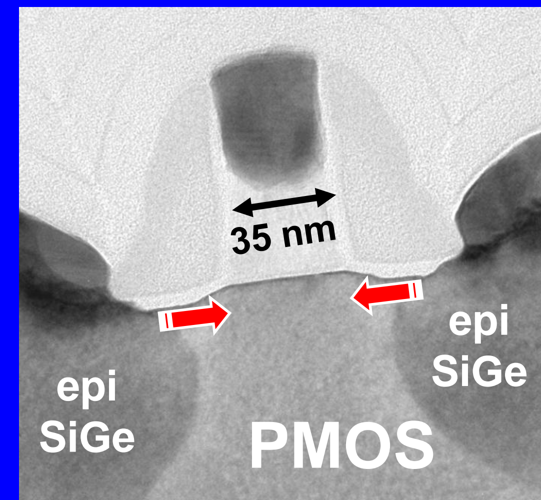
Outline

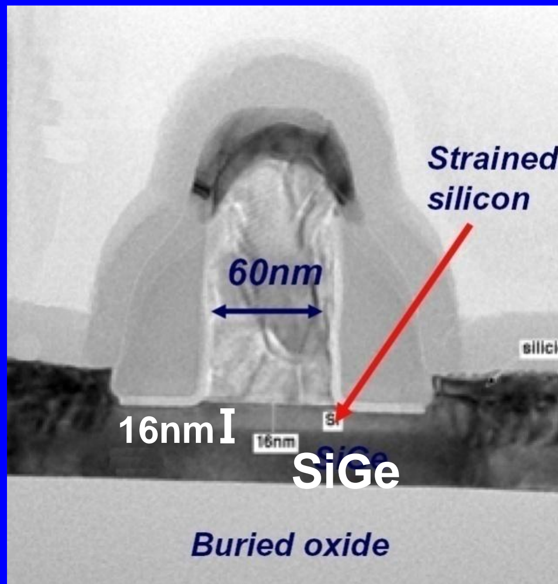
- Motivation
- Modeling of unstrained SiGe
- Modeling of strain effects
- Kinetic Monte Carlo simulations
- Prospects and conclusions

SiGe and Strain in MOSFETs

- **mobility ↑**
- **drive currents ↑**



Tyagi, INTEL, IEDM 05



Lee et al, IEDM 02

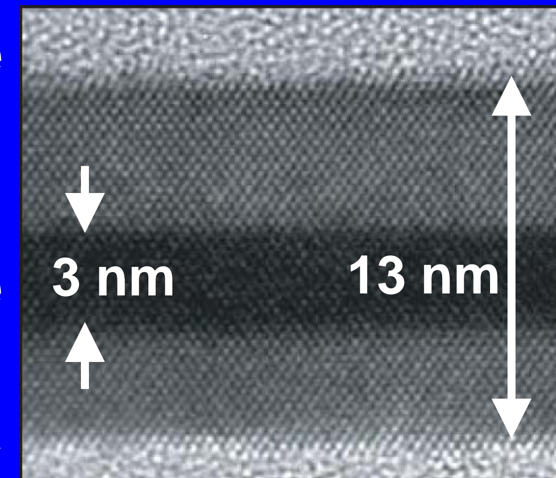
Gate oxide

Strained Si

Strained SiGe

Strained Si

BOX



Antoniadis, IBM J. Res. Dev. 2006

Simulation of SiGe processing

- **New issues: Ge content and strain**
  - **Modification of diffusivities**
  - **Modification of the electronic structure**
  - **Dopant segregation in Si/SiGe**
  - **Si-Ge interdiffusion**
  - **Strain anisotropy and 3D geometries**
- **Drawbacks for continuum simulators:**
  - **Many equations** (many mechanisms, 3D…)
  - **Parameters** (difficult correlation with microscopic properties)

Atomistic Kinetic Monte Carlo (KMC)

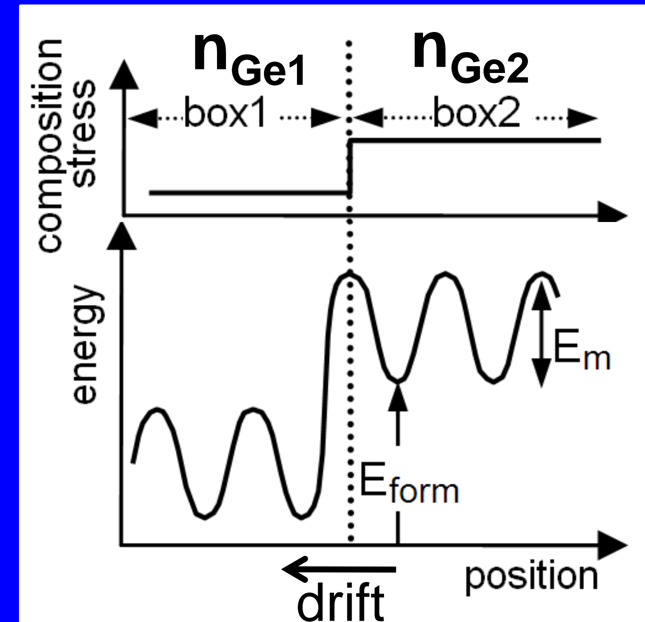
- **Detailed atomistic description of defects and dopants.**
- **Can handle sizes and times for device processing.**
- **Implemented in DADOS (incorporated into *Sentaurus Process Simulator*).**

Features of KMC simulators

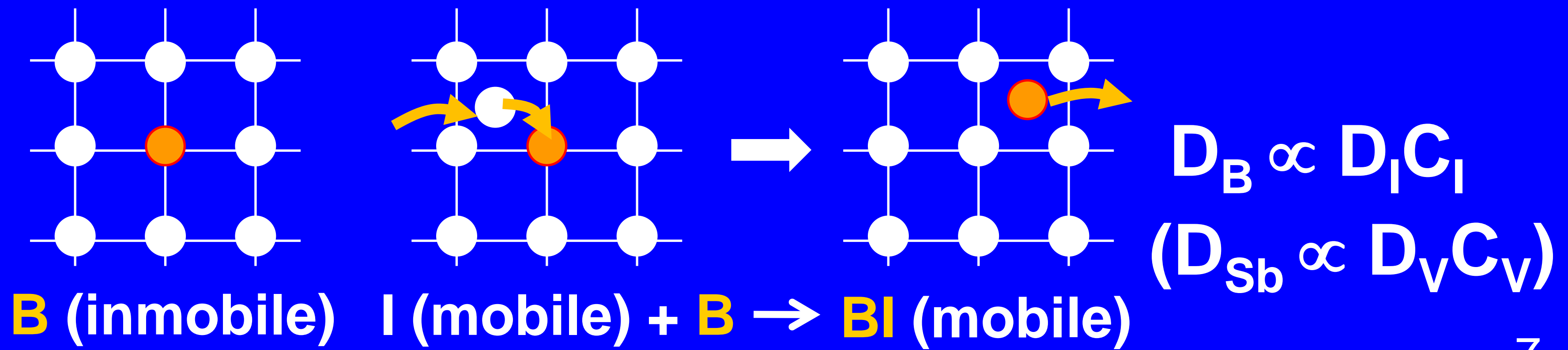
- **Computation time increases moderately with number of mechanisms.**
- **Direct plug of *ab-initio* or basic experimental data.**
- **Inherently 3D.**
- **More advantageous for deep submicron, far from equilibrium,…**

Atomistic diffusion scheme

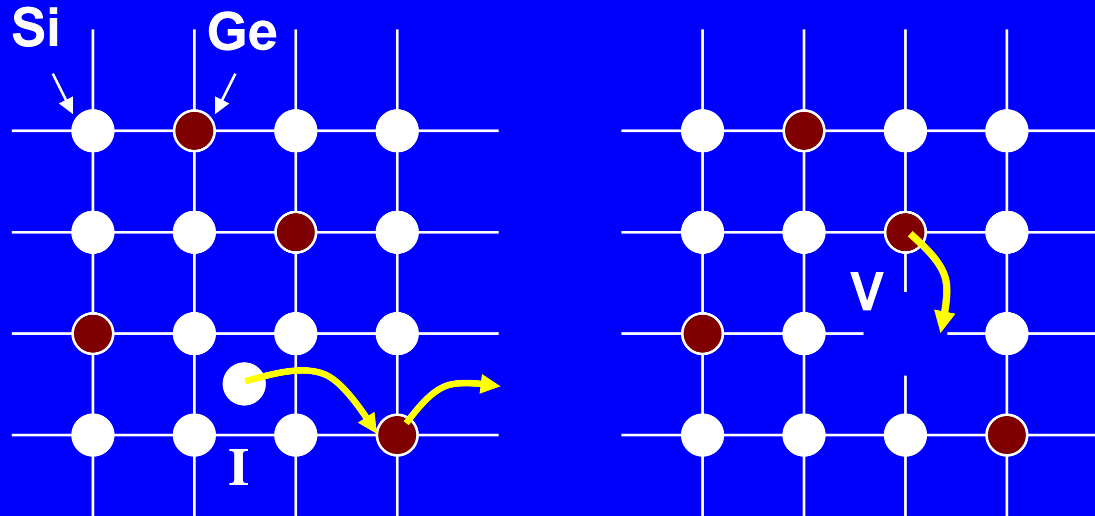
- Ge atom counters per box
- Formation energy (E_{form}): depends on Ge, strain,…
- Jump probability rejection as a function of local ΔE_{form}

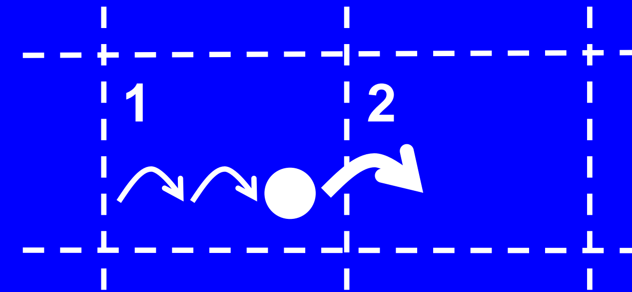


- Dopant diffusion: assisted by defects



Si-Ge interdiffussion scheme





- Also driven by Is & Vs
- I: box1 → box2 $P(Ge_{1\to 2}) \propto n_{Ge1}$
- In SiGe, $D_{Si} \neq D_{Ge} \Rightarrow$

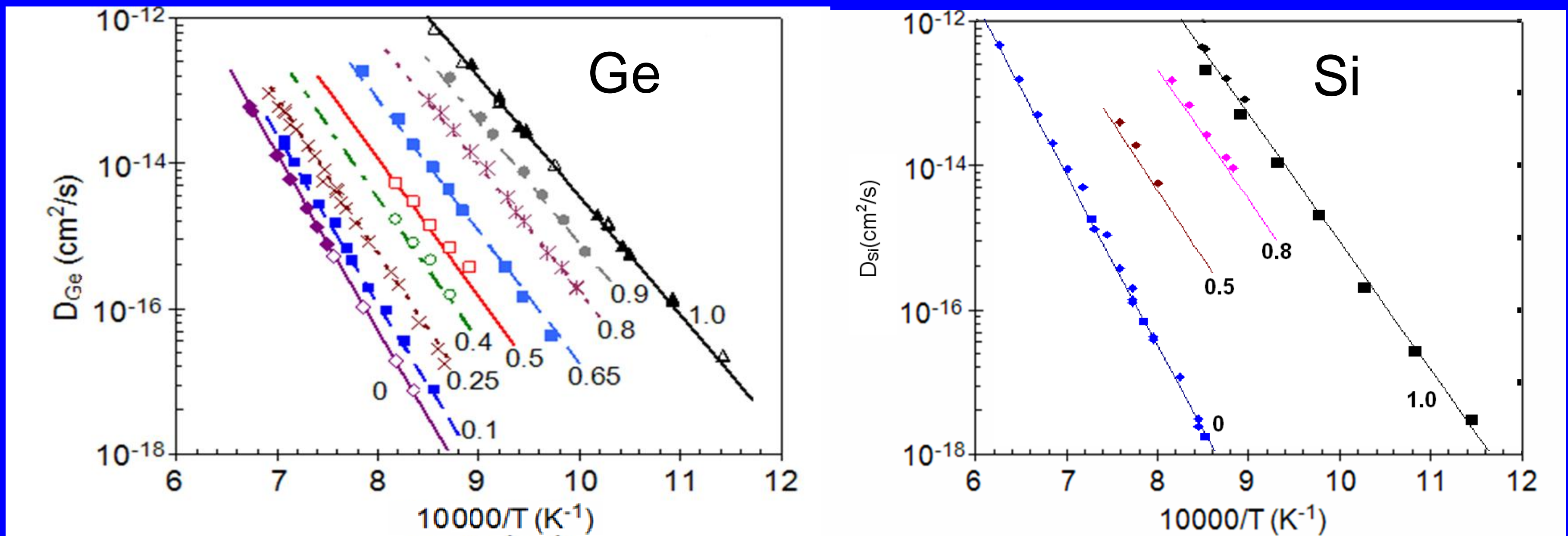
$$P(Ge_{1\to 2}) = \frac{\alpha_I n_{Ge1}}{\alpha_I n_{Ge1} + (n_{at} - n_{Ge1})}$$

- Similarly for Vs.

α_I = Ge/Si transport fraction of an I

Ge and Si self-diffusivities in SiGe

- E and S linear with Ge content: excellent agreement with experimental data.



Experiments: Zangenber et al, 2001; Strohm, 2002; Werner et al,1985; Bracht et al, 1998; Silvestri et al, 2006

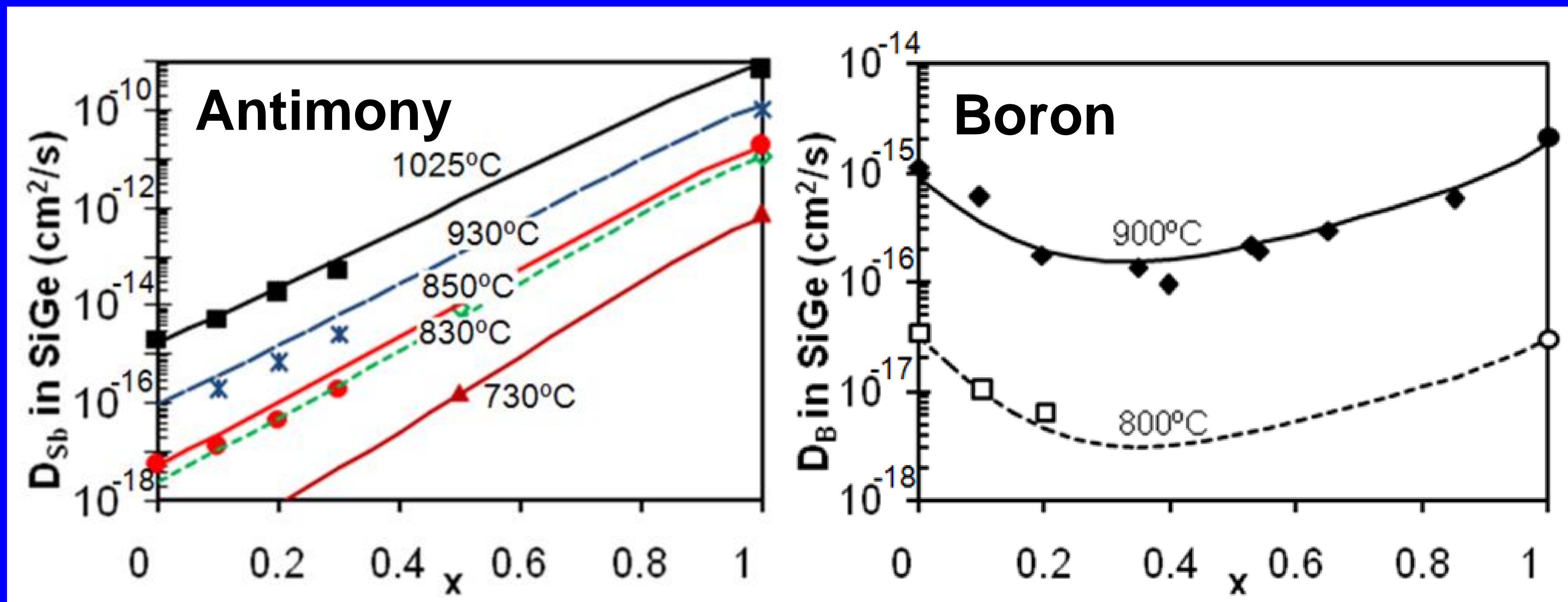
Dopants: diffusion and segregation vs. Ge content

Example: Boron

- **Diffusivity:** $D_B \approx D^0_{Bi} \frac{[BI^0]}{[B^-]}$ **depends on:**
  - **Interstitial transport:** $D_I C_I$
  - $\underbrace{E_m(BI^0) - E_b(BI^-) + (e(BI^-) - E_i)}_{\text{"chemical"}} + \underbrace{(E_i - E_F)}_{\text{"extrinsic"}}$
- **Segregation:**
  - $E_{form}(B^-) = \underbrace{E_{form}(B^0) + (e(B^-) - E_i)}_{\text{"chemical"}} + \underbrace{(E_i - E_F)}_{\text{"extrinsic"}}$
- **No need for B-Ge pair model assumption ready for other dopants.**

Dopants: diffusion in intrinsic unstrained $Si_{1-x}Ge_x$

- Charge levels: quadratic with Ge content
- Good fit to experiments.



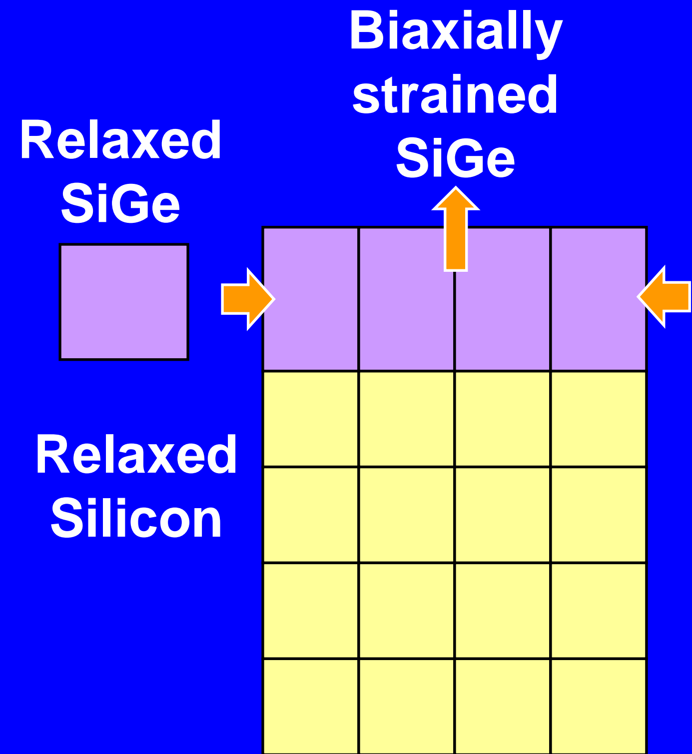
Experiments: Kringhøj et al, 1996; Laitinen, 2004;
Kuo et al, 1995; Uppal et al, 2004

Strain

Example: SiGe on Si

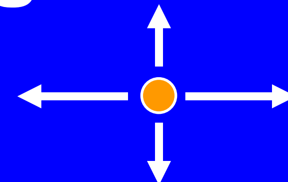
Biaxial strain, equivalent to hydrostatic + uniaxial

Δ vol. < 0 $\varepsilon_{\perp} > 0$



Effects on diffusion:

- $E_{form}(I) \uparrow \Rightarrow D_B \downarrow$
- $E_{form}(V) \downarrow \Rightarrow D_{Sb} \uparrow$
- Changes in band and charge levels $\Rightarrow \Delta D$
- Diffusion jump anisotropy



Dopants in strained SiGe

Example: Boron $D_B \approx D^0_{Bi} \frac{[BI^0]}{[B^-]}$ depends again on:

- $D_I C_I$
- $\underbrace{E_m(B_i^0) - E_b(B_i^-) + (e(B_i^-) - E_i)}_{\text{"chemical"}} + \underbrace{(E_i - E_F)}_{\text{"extrinsic"}}$

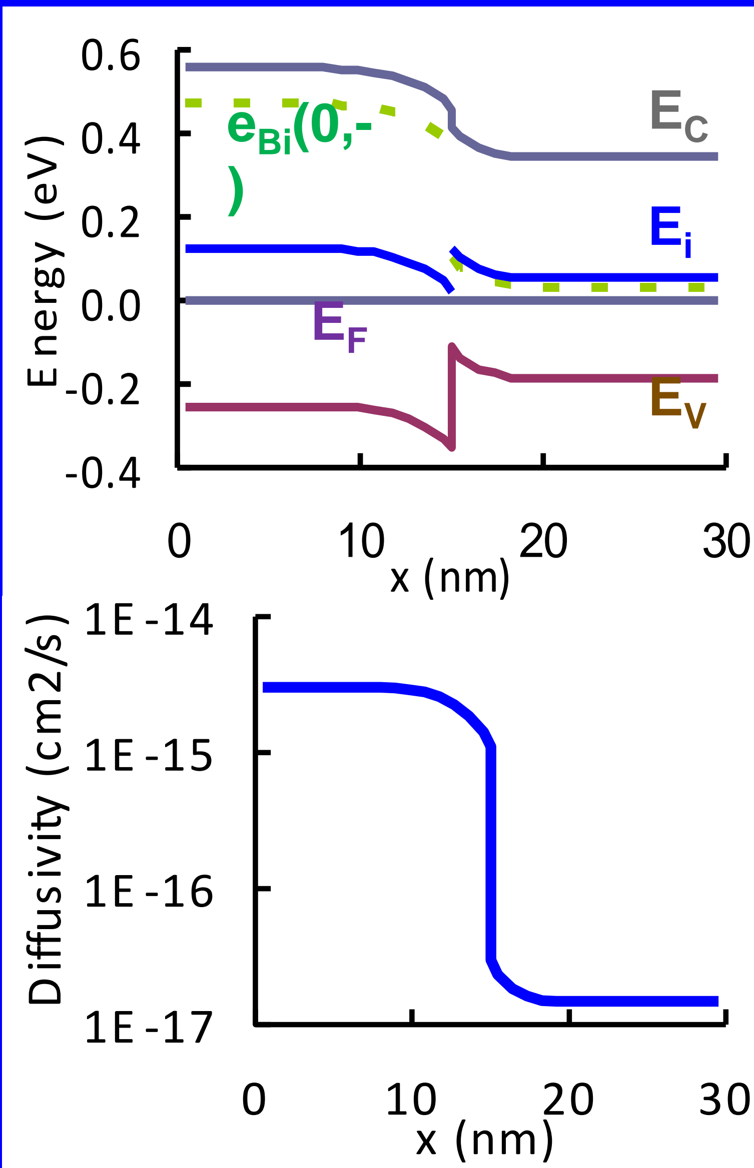
- **Band changes:** hydrostatic + band splitting
- **Charge levels:** assumed proportional to hydrostatic change of E_{gap}

Strain: consequences on extrinsic diffusivity

- **Si/SiGe heterostructure bands at process temperatures**

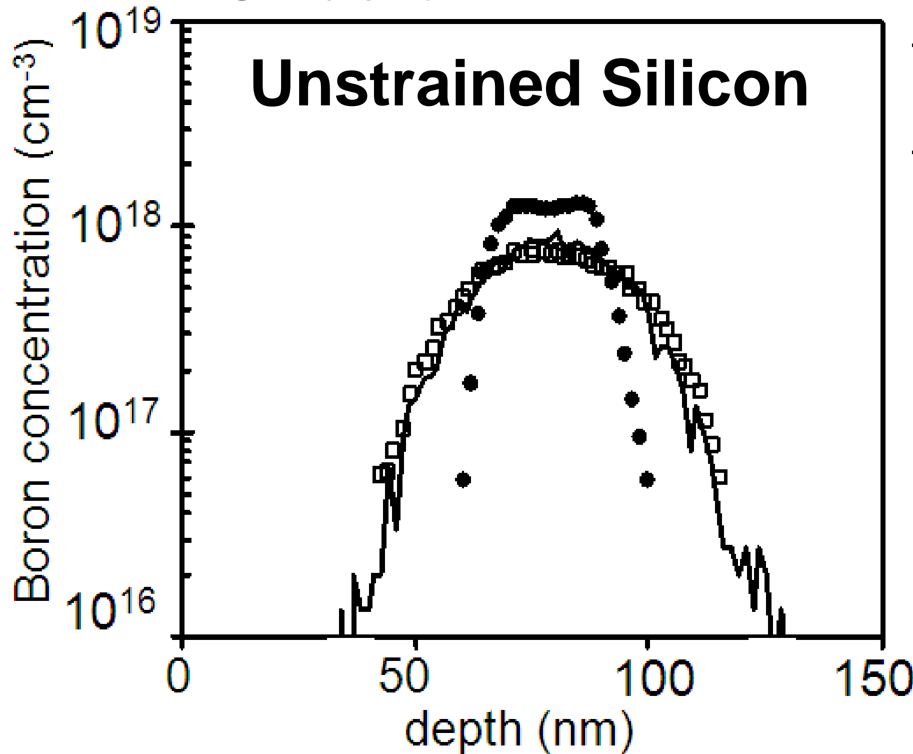
  10^{19} cm^{-3} uniformly B-doped Si/ $Si_{0.7}Ge_{0.3}$ abrupt structure at T = 900°C.

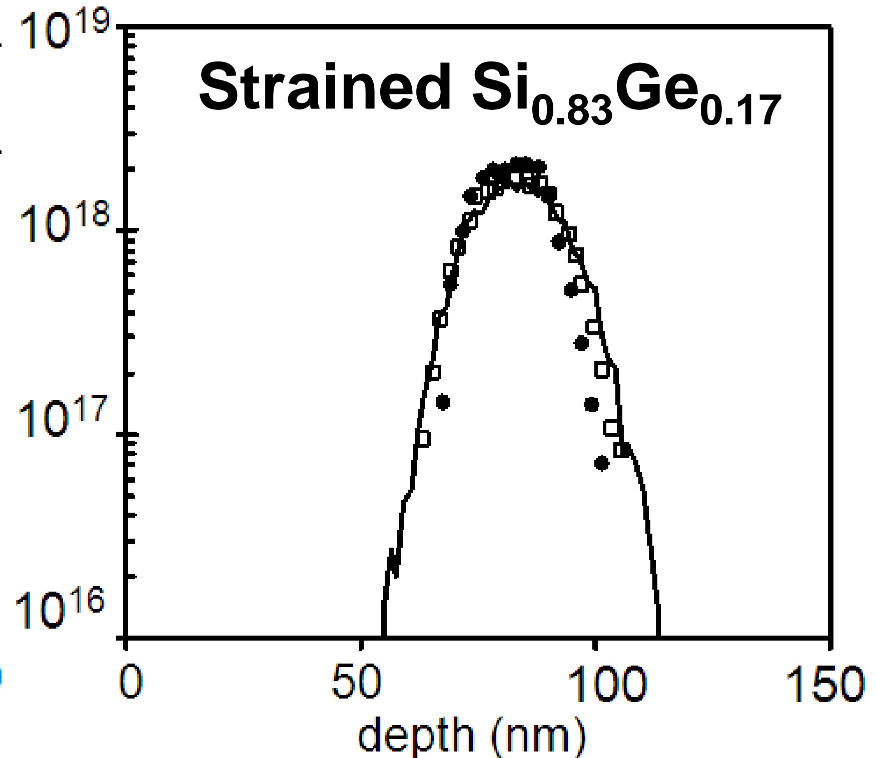
- **Effect of band-bending on extrinsic B diffusivity**



KMC simulations

Boron diffusion: Si vs. SiGe

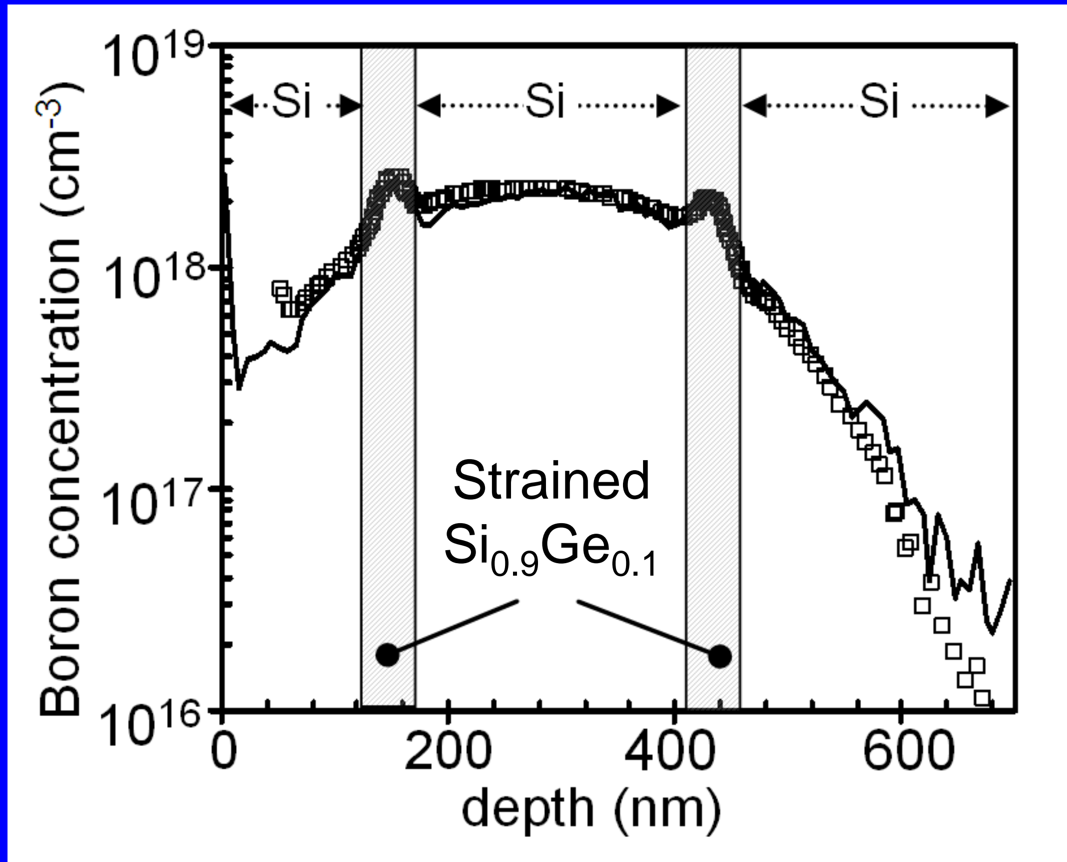




- Retarded by both Ge content and compressive strain

KMC simulations

Boron segregation to SiGe



96 hours at 850°C

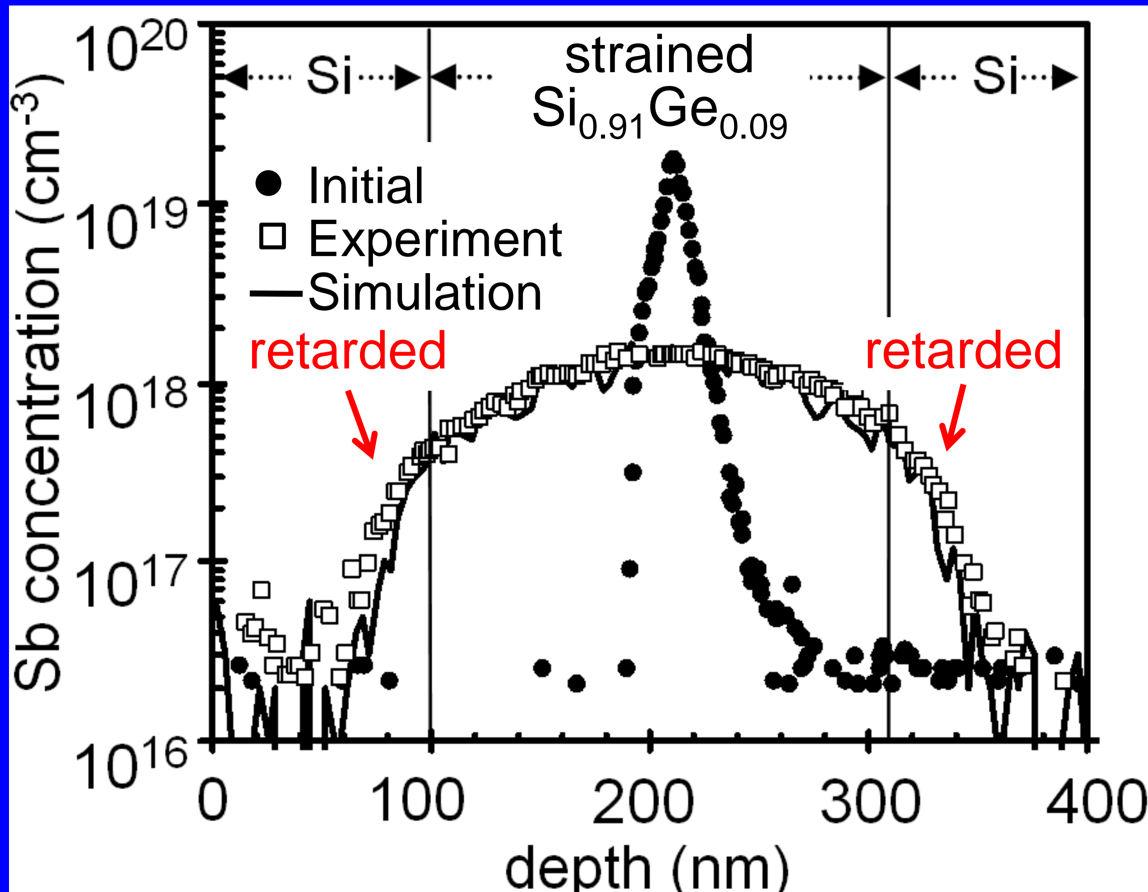
Dots: Experiment
Lines: simulation

- **No assumption of B-Ge pairs**
- **Simultaneous interdiffusion**

Experiment: Lever et al, J. Appl. Phys, 1998

KMC simulations

Antimony diffusion in Si/SiGe/Si structures



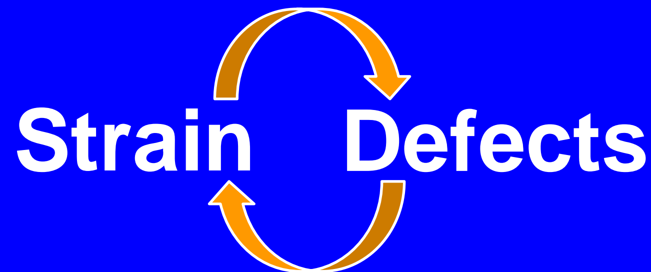
T = 1028ºC
t = 30 min

- **Sb (V-assisted) faster in SiGe due to both Ge and strain**

Experiment: Kringhøj et al, Phys. Rev. Lett, 1996

What's next ?

- Ready for general strain tensors
- Defect-induced strain



- Effect of strain on extended defect transformations

  Example: {311} to Dislocation Loops

Conclusions

- KMC, which is advantageous for the complex structures of ultimate scaled CMOS, can also efficiently account for SiGe composition and strain effects.
- Since it can take microscopic, basic parameters as input, it can be used to test *ab-initio* calculation results.
- Furthermore, it can be used to calibrate continuum-based process simulators.