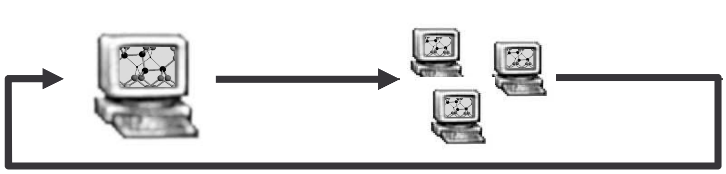


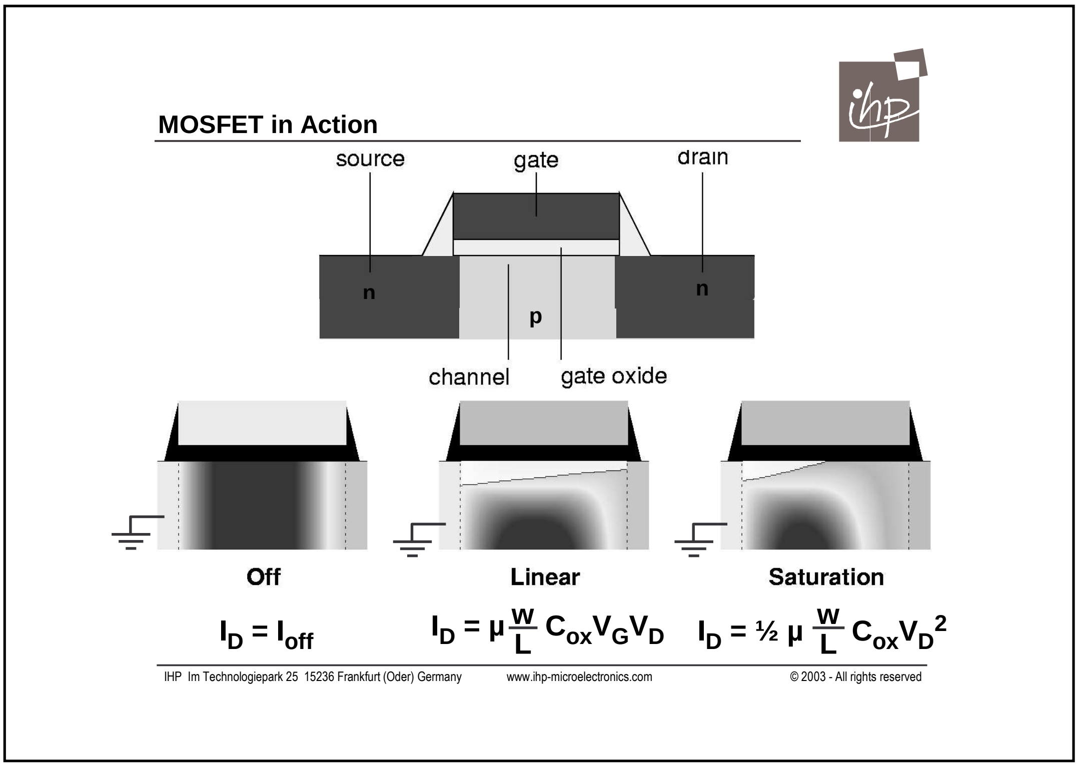
Ab initio Total Energy Calculations for Silicon Microelectronics

Jarek Dąbrowski

IHP
Im Technologiepark 25
15236 Frankfurt (Oder)
Germany

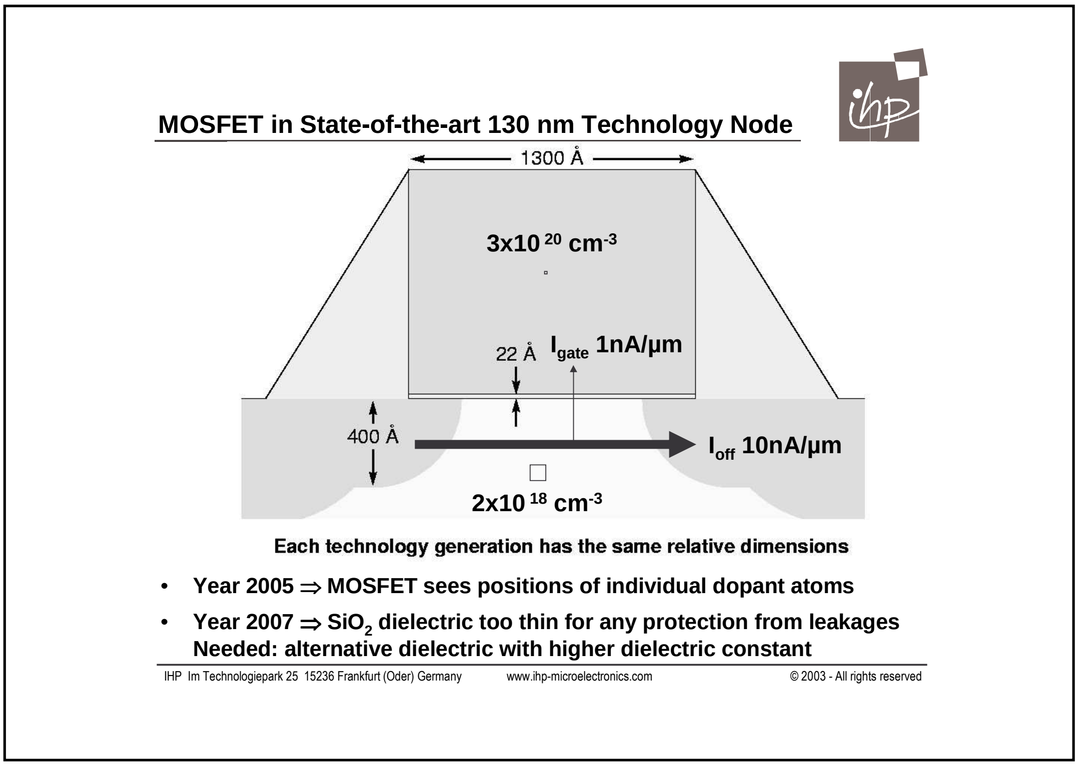
Agenda

- **Introduction**
  CMOS technology and MOS transistor
- **Doping of silicon**
  <u>fhimd example</u>: Charge states of Si interstitials
  <u>fhimd example</u>: Vacancy-assisted diffusion of As
- **High-k dielectrics**
- **<u>fhimd example</u>: Oxidation of the Pr_2O_3/Si(001) interface**
  <u>fhimd example</u>: Interfacial silicate formation in Pr_2O_3 films on Si(001)
- **Summary**



MOSFET in Action

$I_D = I_{off}$ $\quad$ $I_D = \mu \frac{W}{L} C_{ox} V_G V_D$ $\quad$ $I_D = ½ \mu \frac{W}{L} C_{ox} V_D^2$

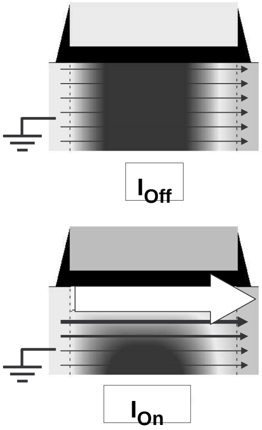


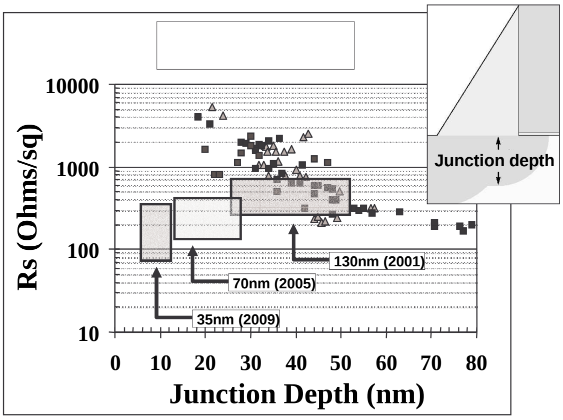
MOSFET in State-of-the-art 130 nm Technology Node

Each technology generation has the same relative dimensions

- **Year 2005 ⇒ MOSFET sees positions of individual dopant atoms**
- **Year 2007 ⇒ SiO_2 dielectric too thin for any protection from leakages Needed: alternative dielectric with higher dielectric constant**

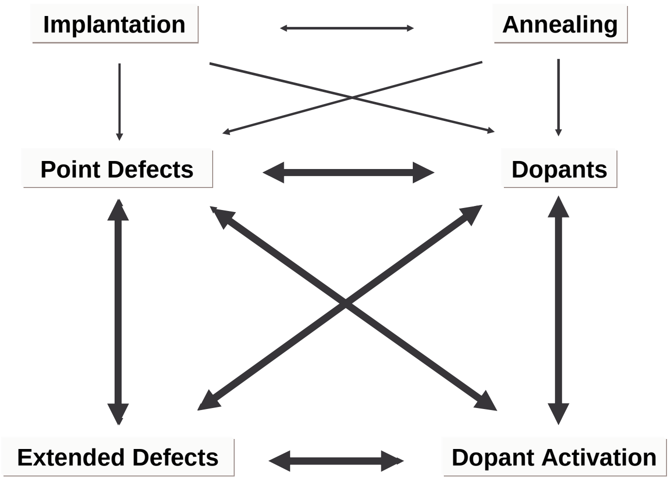
Key Issue: Junction Depth





- Dopant activation ⇒ annealing ⇒ diffusion ⇒ profile broadening
  Needed: better intuition about dopant-defect interaction!

Everything Is Interconnected...



Implantation

Annealing

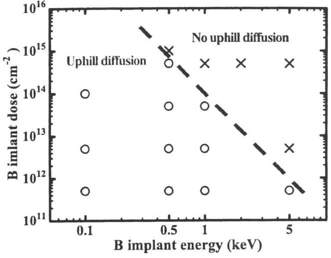
Point Defects

Dopants

Extended Defects

Dopant Activation

H. Tsuji et al., IEDM, 2002



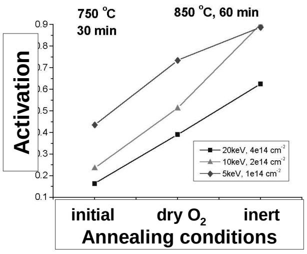
Some of the Unresolved Issues

- **How and why is defect evolution affected:**
  - by substrate type (Fermi level effects)
  - by annealing ambient (point defect type)
  - by ramp rates (activation energies)
- **Interactions between dopants and point defects**
  Relative importance of Si_i - and Si_V -mediated diffusion for P, As, Sb
  BIC: B activation is expected to be improved by Si_i, not hindered!
  Influence of F on B diffusion in amorphous Si
- **Interactions between point and extended defects**
  Effect of point defect background on stability of extended defects
  Structures and energies of small clusters of Si interstitials
  Dependence of point defect background on implantation energy
  Transition of small interstitial clusters to {113} defects
- **Interactions between dopants and extended defects**
  “Surface proximity” effect on dopant diffusion
  Segregation of dopants to SiO_2/Si(001) interfaces

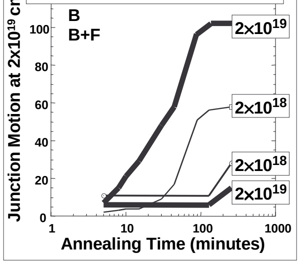
© 2003 - All rights reserved

Some of the Unresolved Issues - figures

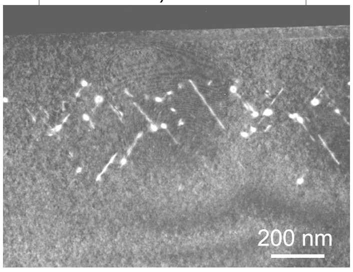
A. D. Lilak et al., APL, 2002



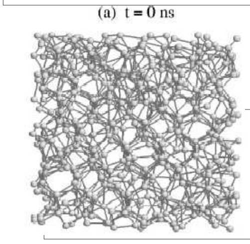
J. M. Jacques et al., MRS 2002



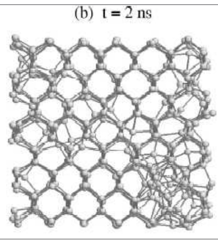
F. Cristiano, CHiPPS-2002



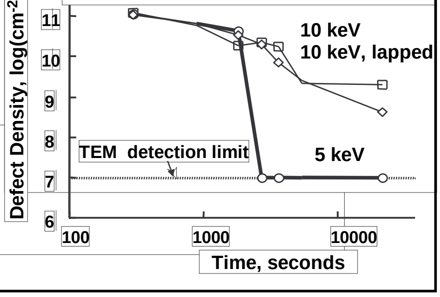
G. H. Gilmer et al., PRB 2001



G. H. Gilmer et al., PRB 2001

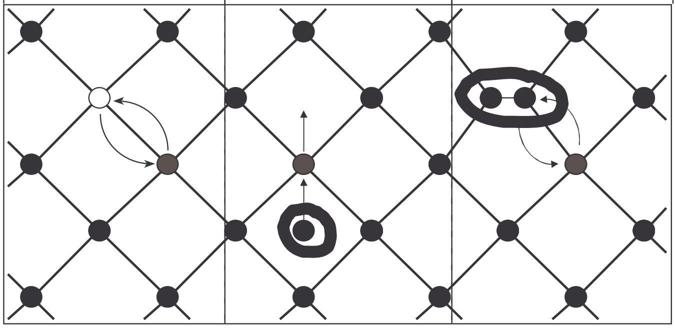


A. King, MS Thesis, Florida Univ. 2003



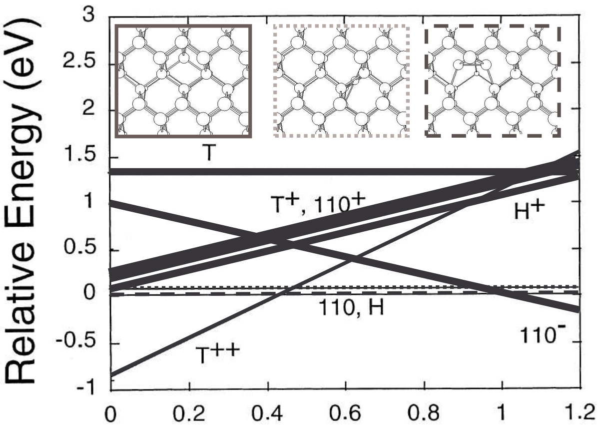
Defect-mediated Diffusion Mechanisms

Vacancy mechanism $D + V \Leftrightarrow DV$	Interstitial mechanism $D + I \Leftrightarrow D_I$	Interstitialcy mechanism $D + I \Leftrightarrow DI$



● Dopant atom ● Silicon atom

Towards Diffusion Mechanisms: Si_i and Fermi Level



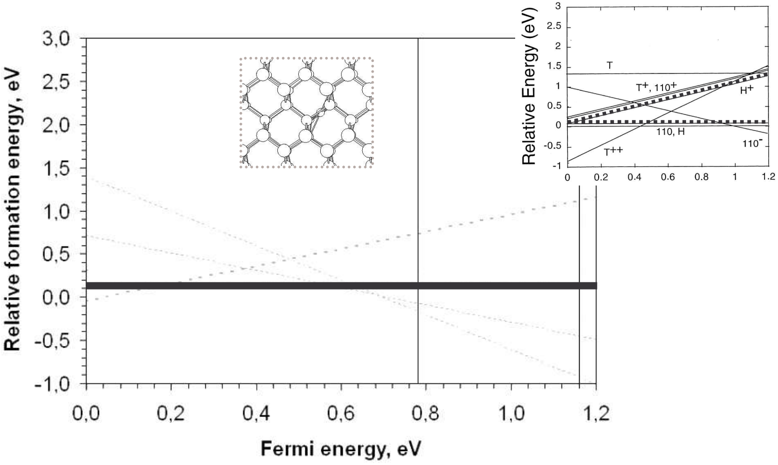
- **Do we REALLY know what are the energies of these interstitials: T(0), T(+), H(+), 110(+), 110(-) ?????**

J. Zhu, Comp. Mat. Sci, 1998

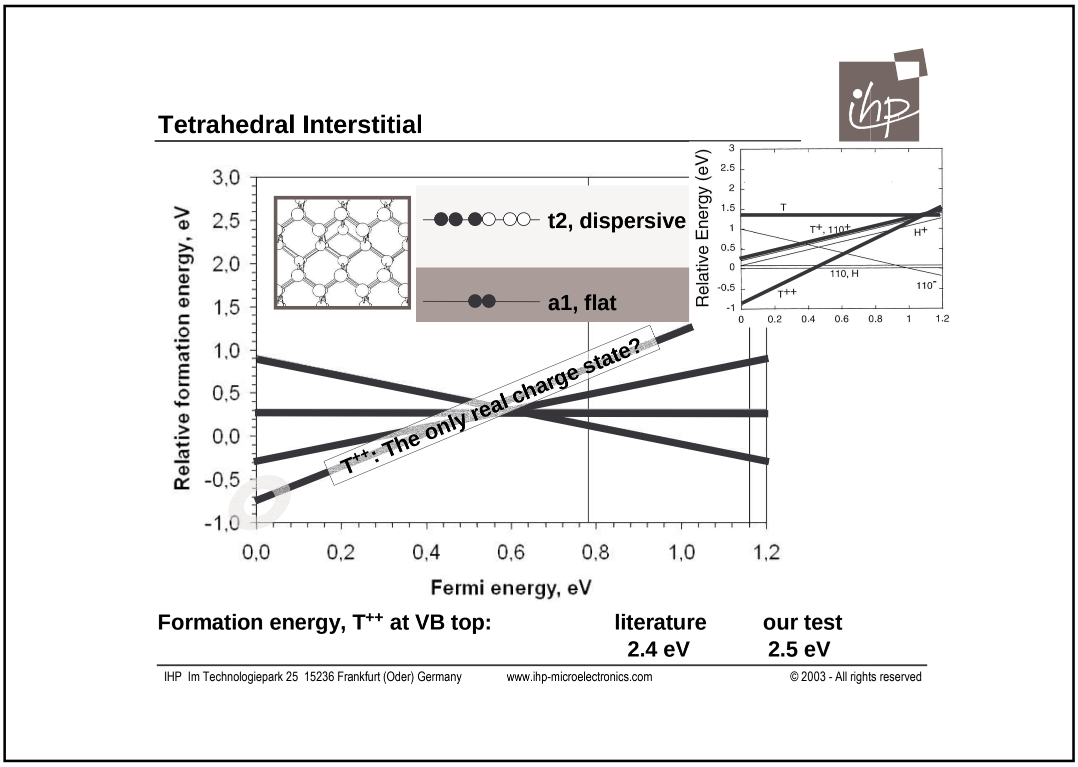
Set up simple test calculation...

Energy cutoff:	**8 Ry**
Cell size:	**4x4x4 (129 atoms)**
Brillouin zone sampling:	**Γ**

Hexagonal Interstitial



Formation energy, H^0:	**literature**	**our test**
	3.5-3.3 eV	**3.3 eV**

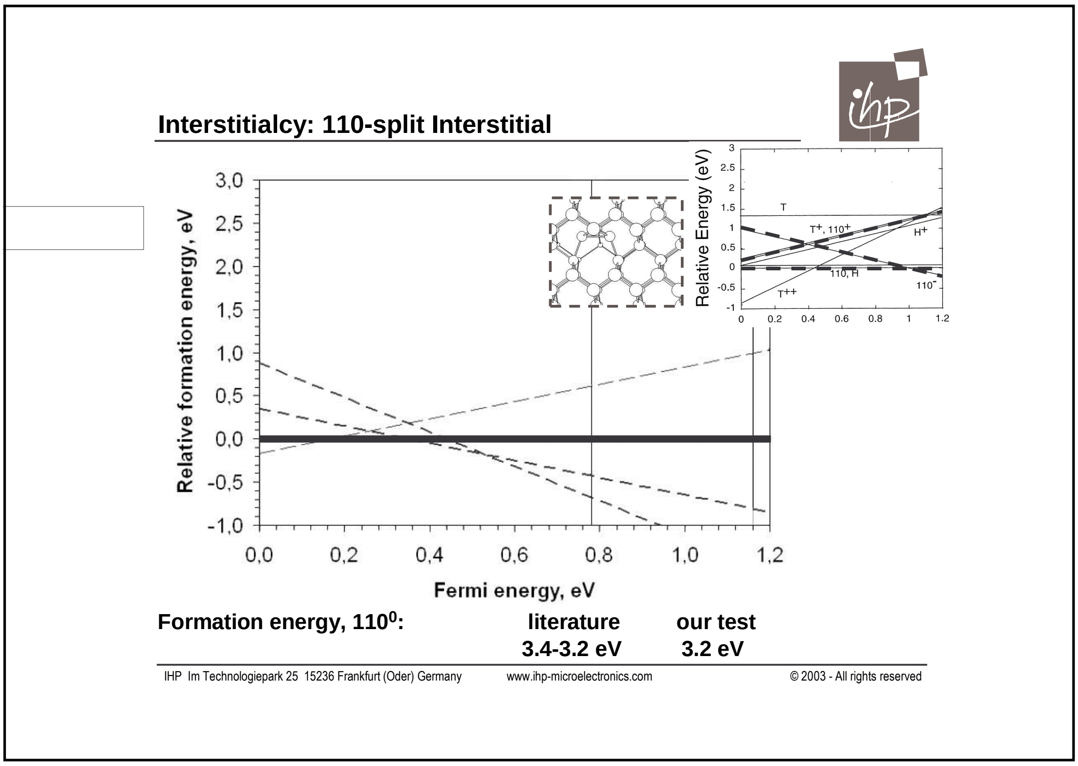


Tetrahedral Interstitial

T^{++}: The only real charge state?

Formation energy, T^{++} at VB top: **literature** **2.4 eV** **our test** **2.5 eV**

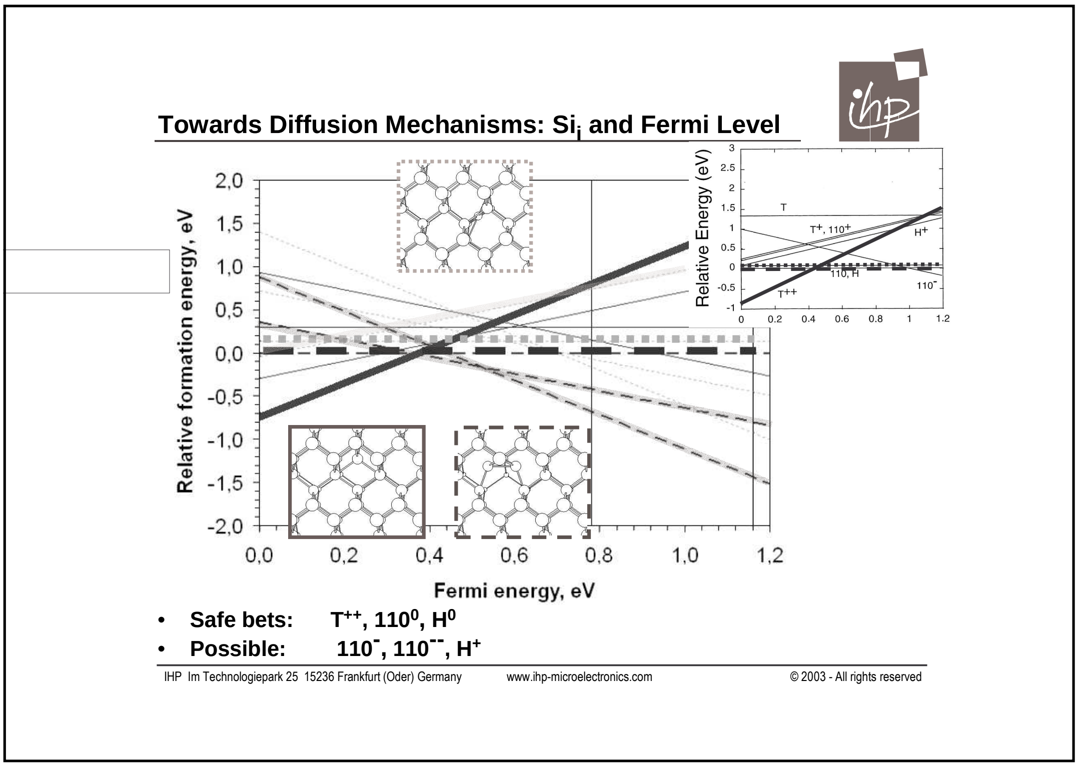
© 2003 - All rights reserved



Interstitialcy: 110-split Interstitial

Formation energy, 110^0: **literature** **3.4-3.2 eV** **our test** **3.2 eV**

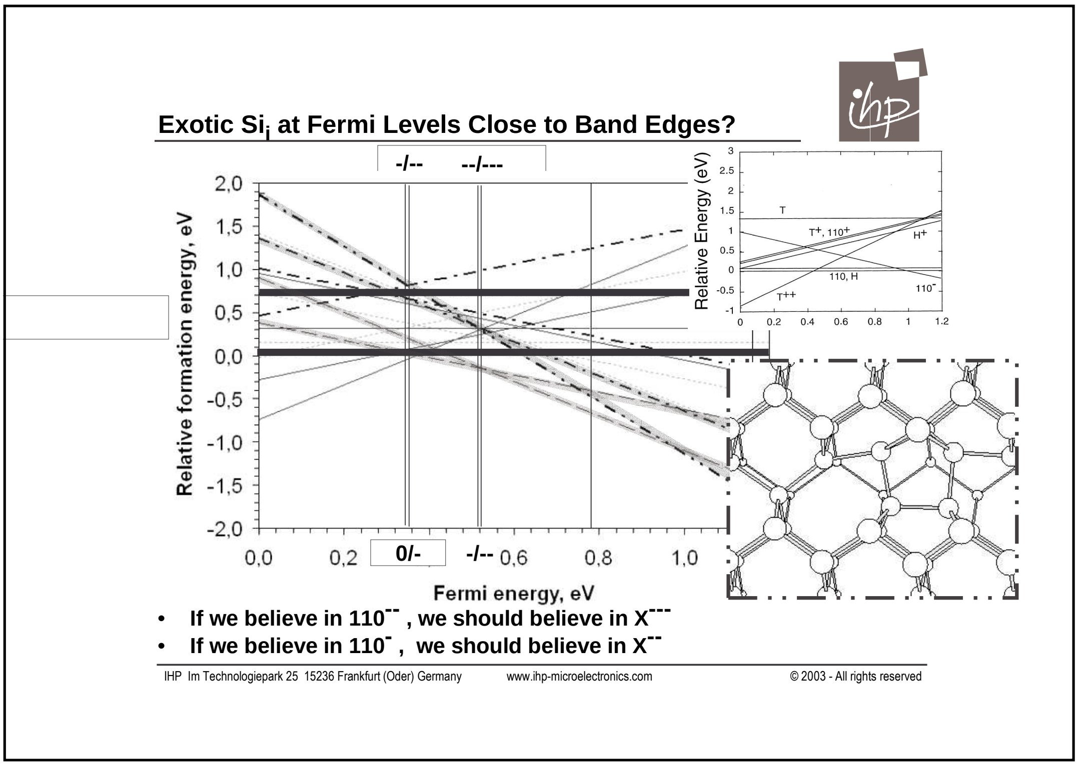
© 2003 - All rights reserved



Towards Diffusion Mechanisms: Si$_i$ and Fermi Level

- **Safe bets:** T^{++}, 110^0, H^0
- **Possible:** 110$^-$, 110^{--}, H$^+$

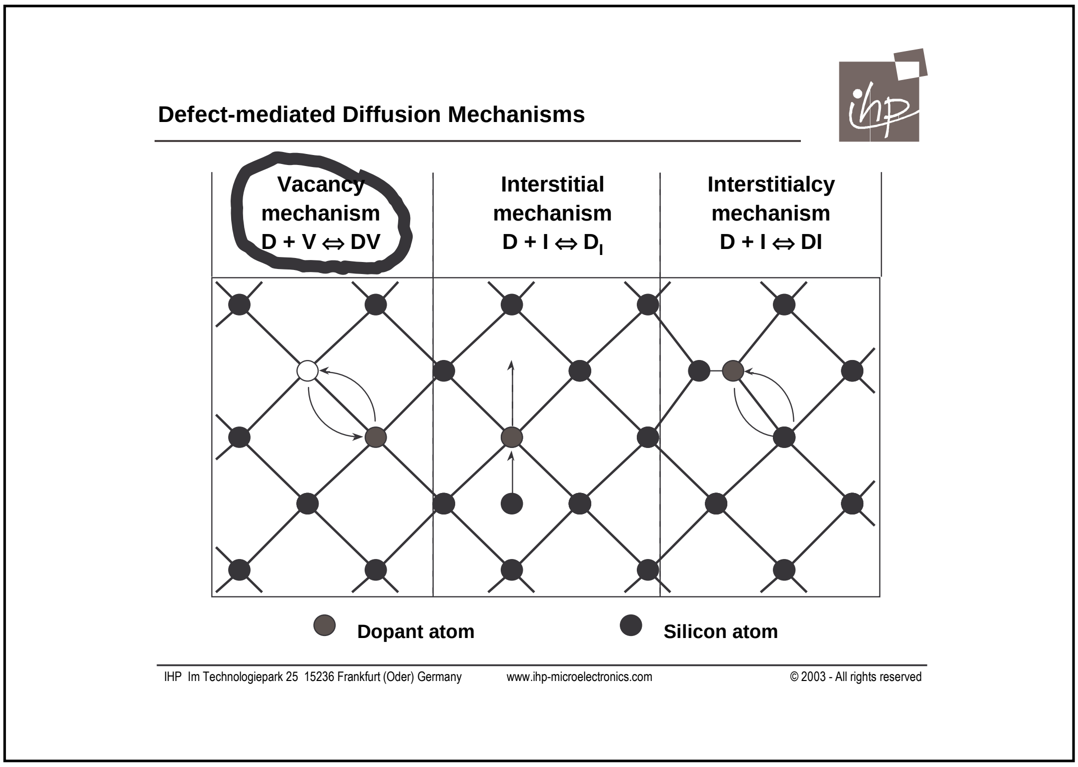
IHP Im Technologiepark 25 15236 Frankfurt (Oder) Germany www.ihp-microelectronics.com © 2003 - All rights reserved



Exotic Si$_i$ at Fermi Levels Close to Band Edges?

- **If we believe in 110^{--} , we should believe in X^{---}**
- **If we believe in 110$^-$, we should believe in X^{--}**

IHP Im Technologiepark 25 15236 Frankfurt (Oder) Germany www.ihp-microelectronics.com © 2003 - All rights reserved

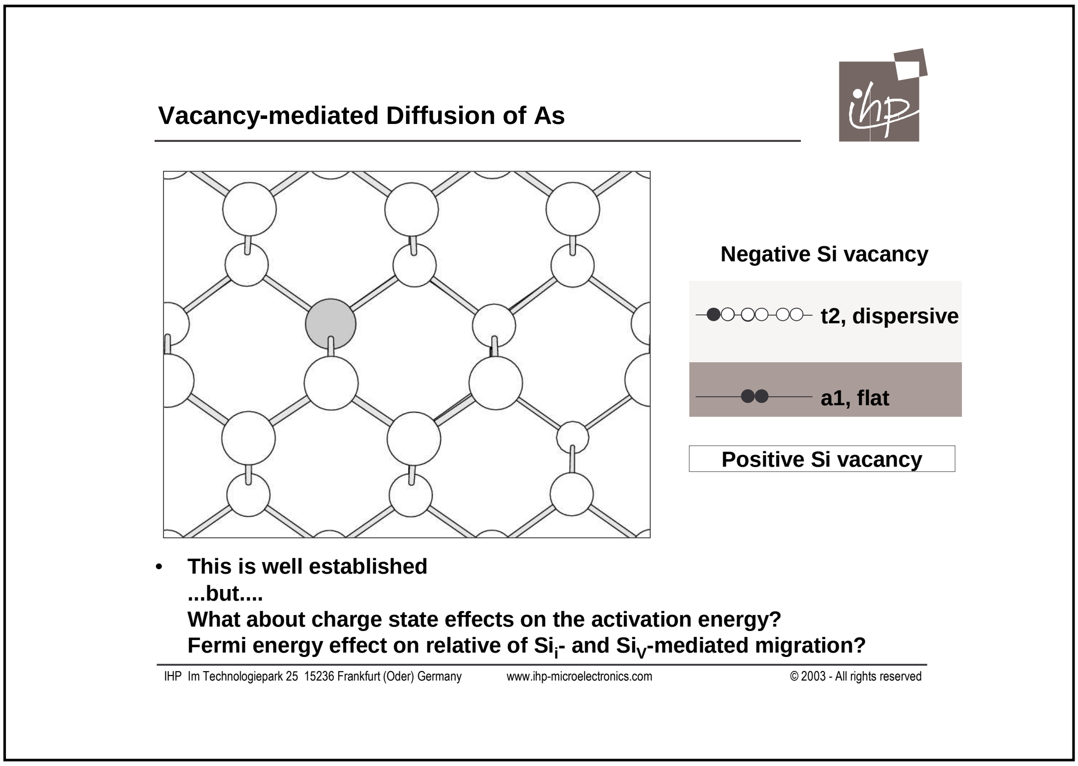


Defect-mediated Diffusion Mechanisms

Vacancy mechanism D + V ⇔ DV	Interstitial mechanism D + I ⇔ D_I	Interstitialcy mechanism D + I ⇔ DI

● Dopant atom

● Silicon atom



Vacancy-mediated Diffusion of As

Negative Si vacancy

t2, dispersive

a1, flat

Positive Si vacancy

- This is well established
  ...but....
  What about charge state effects on the activation energy?
  Fermi energy effect on relative of Si_i- and Si_V-mediated migration?

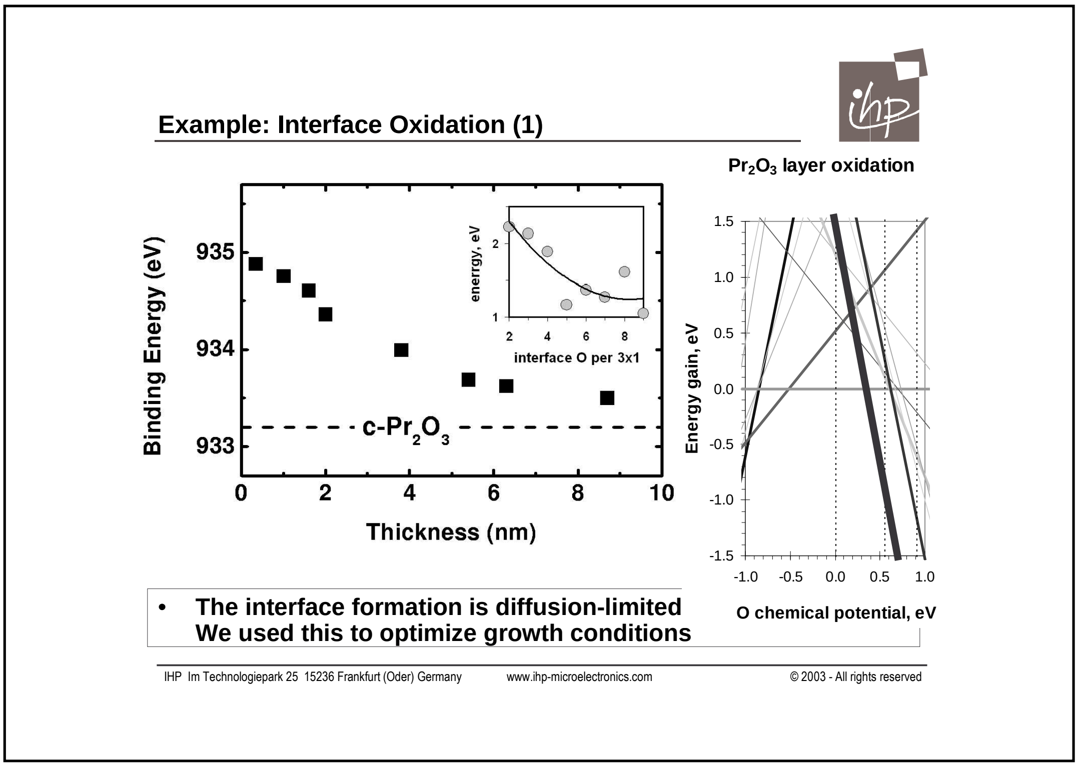
Doping Issues of Potential Interest to Us

- How and why is defect evolution affected:
  - by substrate type (Fermi level effects)
  - by annealing ambient (point defect type)
  - by ramp rates (activation energies)
- Interactions between dopants and point defects
  Diffusion: Si_i versus Si_V mechanism at various Fermi energies
  Clustering: is the BIC model correct?
  Amorphous Si: influence of F on B diffusion
- Interactions between point and extended defects
  Implantation: which point defects are created, how and when?
  Annealing: small Si_i clusters and transition to {113} defects
- Interactions between dopants and extended defects
  Shallow implantation: "surface proximity" effect on dopant diffusion
  Boundary conditions: segregation of dopants to SiO_2/Si(001) interfaces

---

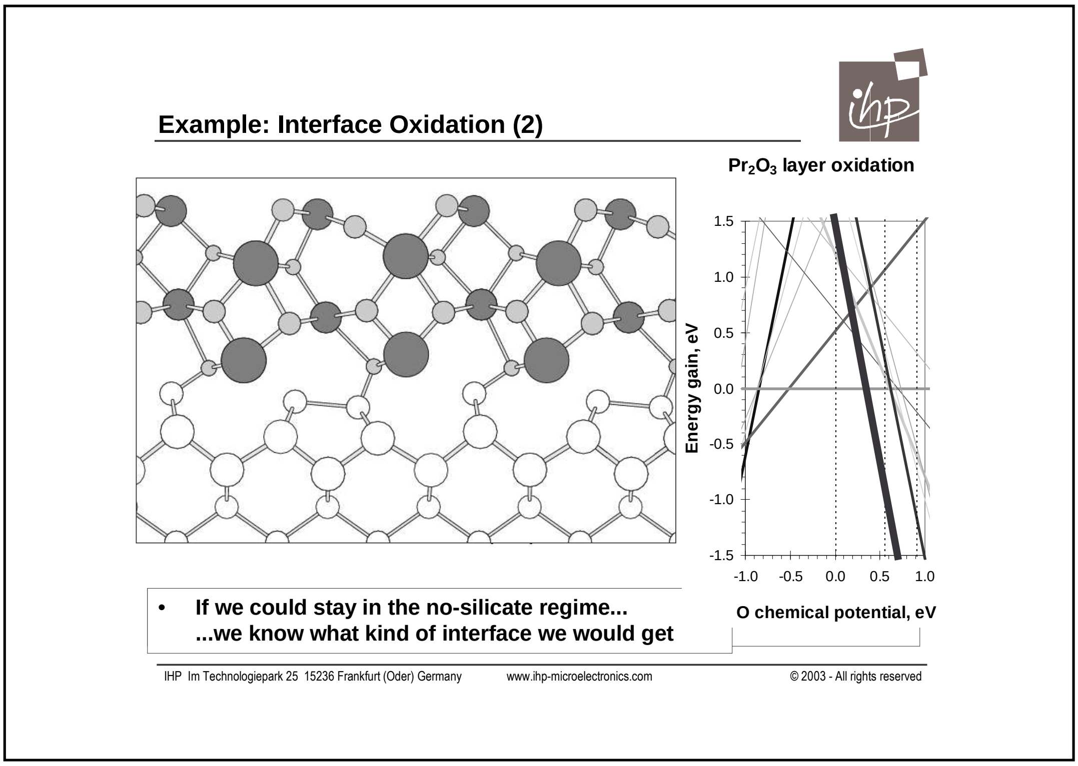
Interface Between Pr_2O_3 and Si(001)

- Pr_2O_3 gate dielectric may be ~8 times thicker than SiO_2!
- Where is the problem?
  Dipole moment ⇒ band offsets change ⇒ gate leakage affected
  Defects form there ⇒ charge is trapped ⇒ bands bend ⇒ V_T changes
  Materials may intermix ⇒ material properties change
  Technologists spoiled by next-to-perfect SiO_2/Si(001) interface...
- What did we learn?
  [redacted]
  Thumb rules for electron counting and energy estimates
- What are the implications?
  Intuitive understanding of the system facilitates experimental work
  Solid basis for future studies



Example: Interface Oxidation (1)

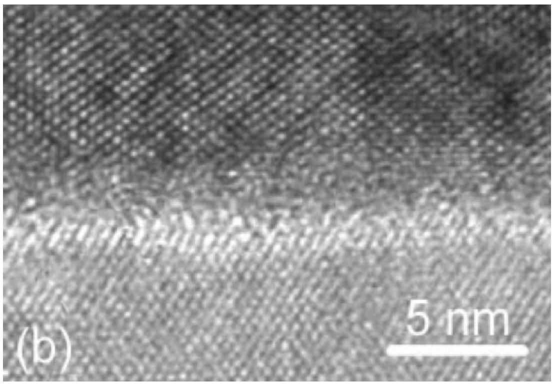
- **The interface formation is diffusion-limited We used this to optimize growth conditions**



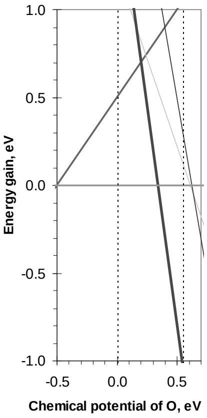
Example: Interface Oxidation (2)

- **If we could stay in the no-silicate regime... ...we know what kind of interface we would get**

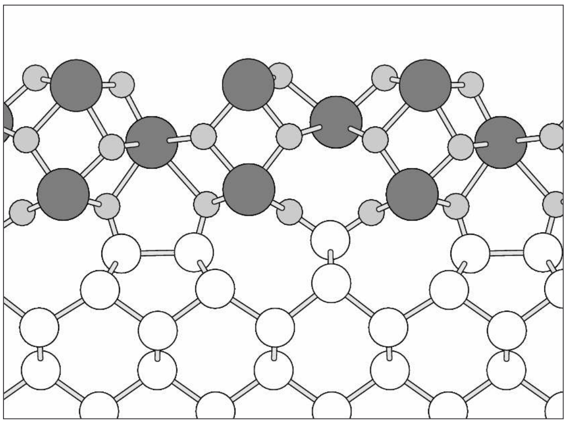
Example: Formation of Interfacial Silicate



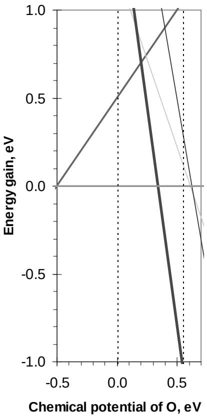
Pr_2O_3 layer oxidation



Example: Formation of Interfacial Silicate



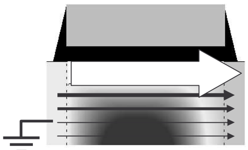
Pr_2O_3 layer oxidation



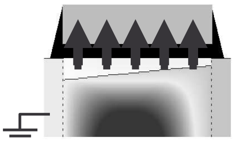
- **GOOD NEWS: IL formation linked to O supply**
- **BAD NEWS: IL contains strained Si-Si bridges**

Summary and Outlook

- **Junction leakage ⇒ implantation, diffusion and activation**
  Diffusion in amorphous Si (B-F interaction?)
  Point defects created during/after implantation
  “Surface proximity” effects (implant energy effects)
  Fermi level effects (charge states vs. diffusion?)
  Clusters of dopants and point defects (BIC model?)
  Pathway from small clusters to {113} defects



- **Gate leakage ⇒ high-k dielectrics**
  Origin of defects, mostly at the interface
  Mechanism of leakage and charge capture
  Band offsets to silicon
  Formation of interfacial oxide
  Formation of interfacial silicate
  Chemical reactions during CVD



$$I_D = \mu \frac{W}{L} C_{ox} V_G V_D$$

Thanks are due to…

• **NIC Jülich**	**Cray T3E time**
• **Victor Zavodinsky**	**Praseodymium pseudopotentials**
• **Dieter Schmeißer**	**Synchrotron radiation studies**
• **Hans-Joachm Müssig**	**Pr_2O_3 film growth**
• **Andreas Fissel**	**Pr_2O_3 film growth**
• **Mark Law**	**Questions on boron, surface proximity**
• **Fuccio Cristiano**	**Questions on extended defects**
• **Wojtek Dąbrowski**	**Animations**