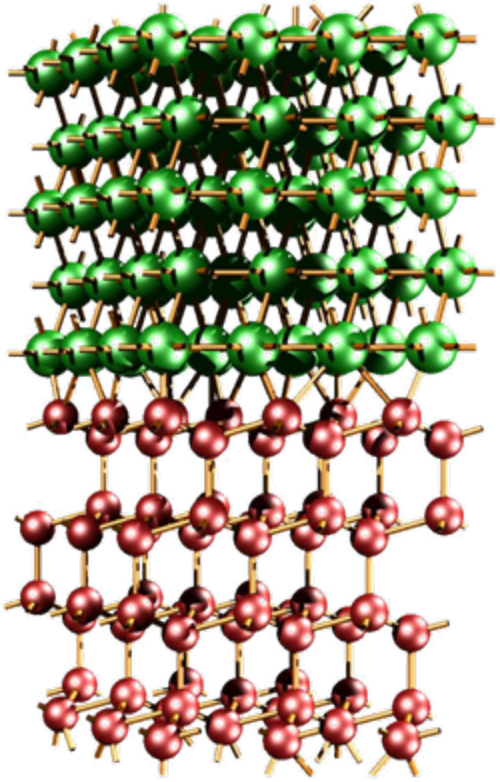
Silicide Formation at the Si-Ti Interface



(in collaboration with TUC group of Prof. Schreiber)

References:

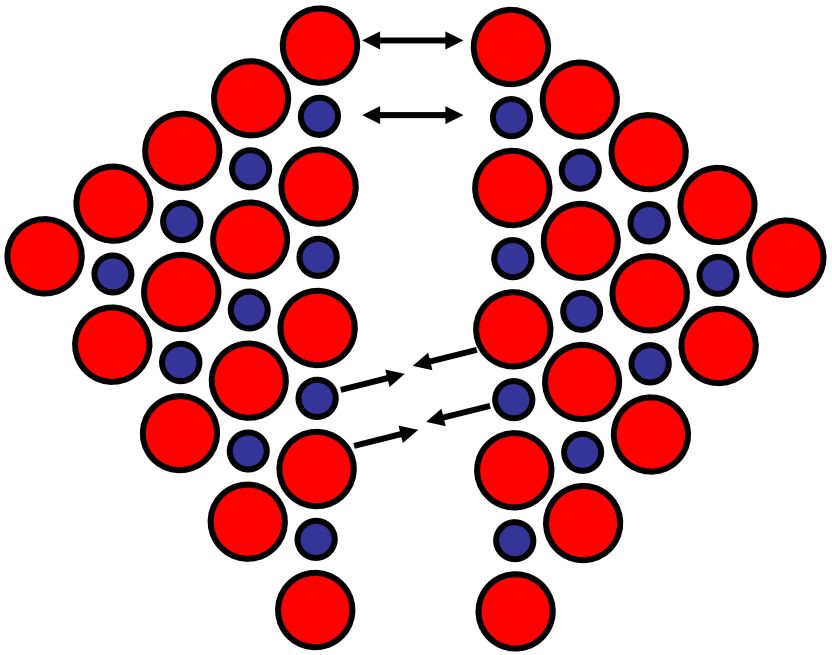
S. Gemming, M. Schreiber, J.-B. Suck: Materials for Tomorrow, Berlin - Heidelberg - New York: Springer, 2007, 978-3-540-47970-3.

S. Gemming, M. Schreiber, “Theoretical investigation of interfaces“, ibid., 91-122.

S. Gemming, A. Enyashin, M. Schreiber, “Amorphisation at Heterophase Interfaces“, in: Karl Heinz Hoffmann, Arnd Meyer: Parallel Algorithms and Cluster Computing - Lecture Notes in Computational Science and Engineering, Berlin - Heidelberg - New York: Springer, 2006, 3-540-33539-0, 235-254.

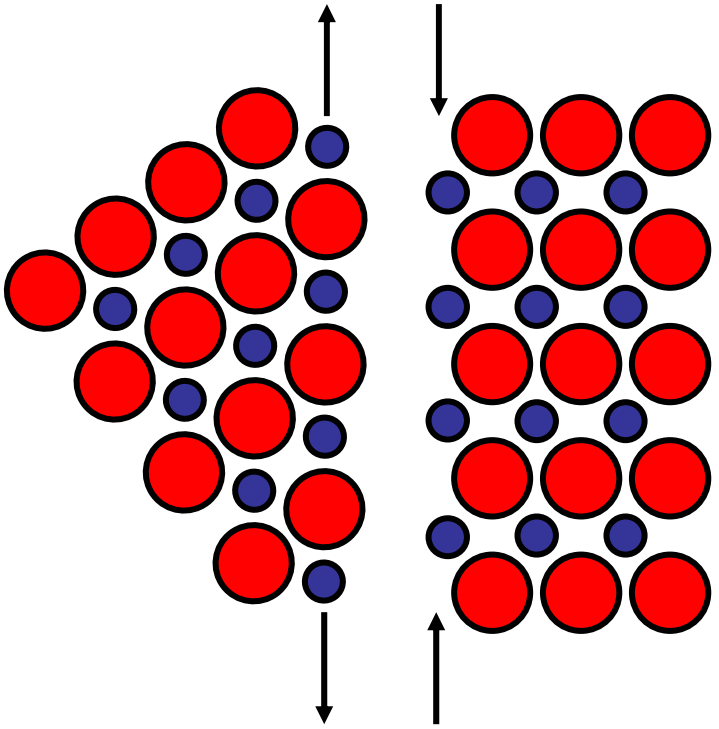
Interfacial interactions

Ionicity
Coulomb interaction



Translation state

Lattice mismatch ν
Elastic stress

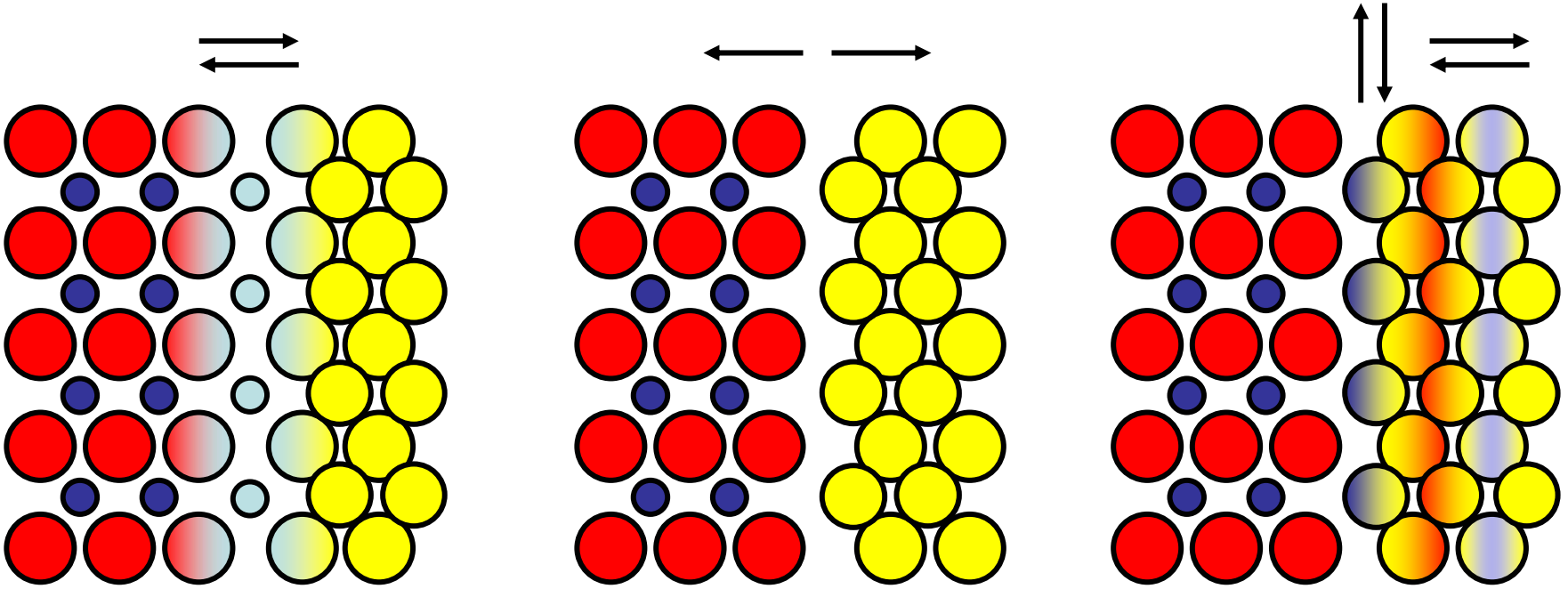


Misfit dislocations

Heterophase interactions

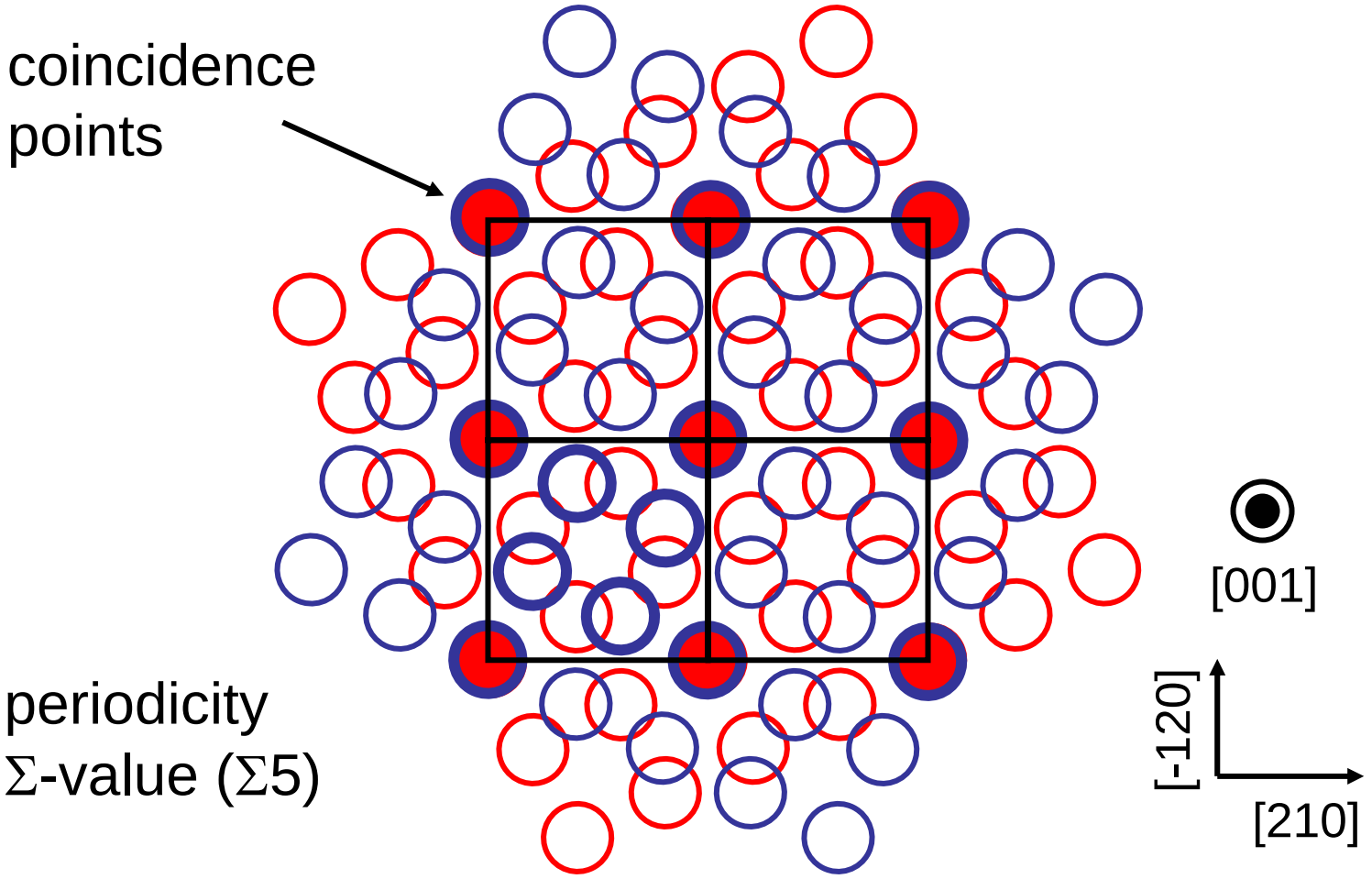
Coulomb + Stress +

e⁻-Transfer + Pauli repulsion + Induced dipoles

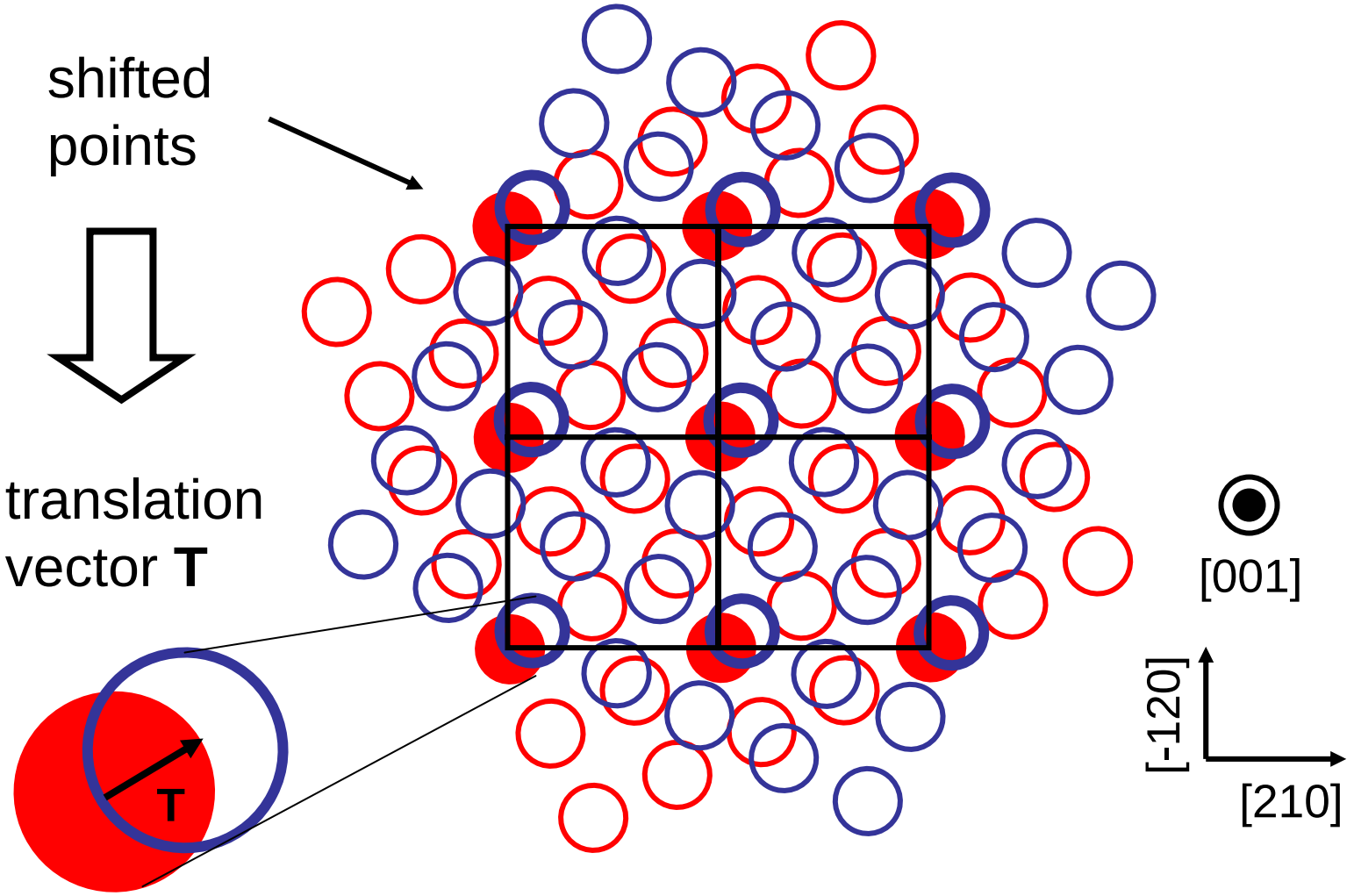


Electronegativity χ | e⁻-Density r_s | Image charges

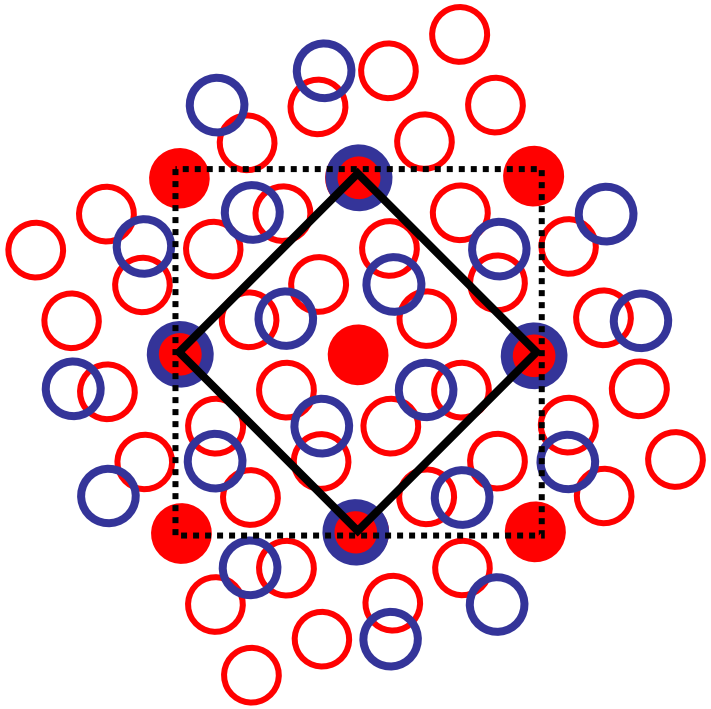
Coincidence site lattice - CSL

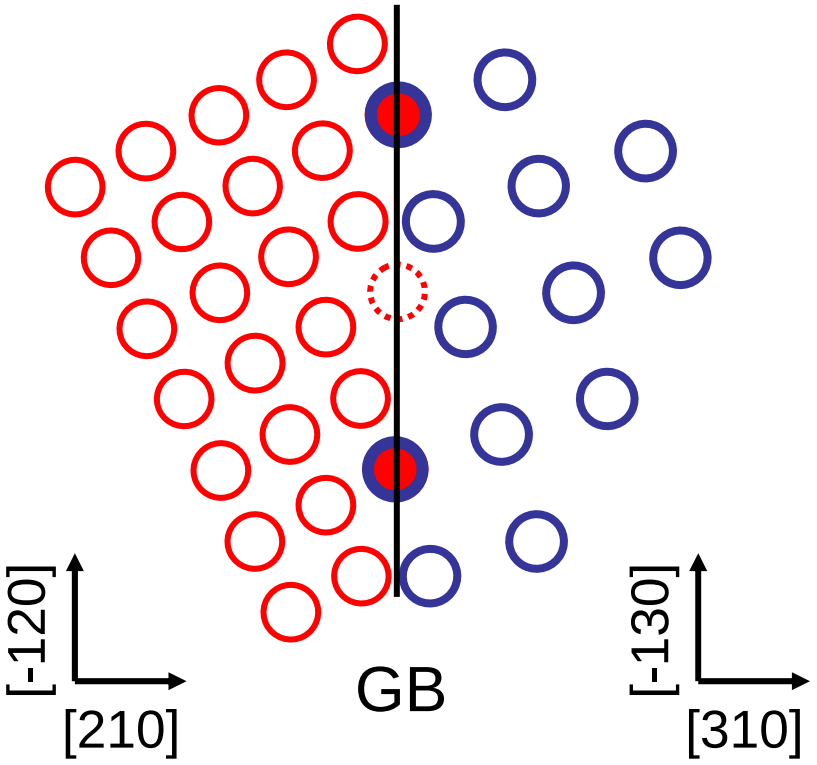


Translation state



Heterophase CSL





area density

$M_1 : M_2 = 10 : 5$

lattice mismatch ν

$a_1 : a_2 = 1 : \sqrt{2}$

$M_1(210) \mid M_2(310)$

$M_1[-120] \parallel M_2[-130]$

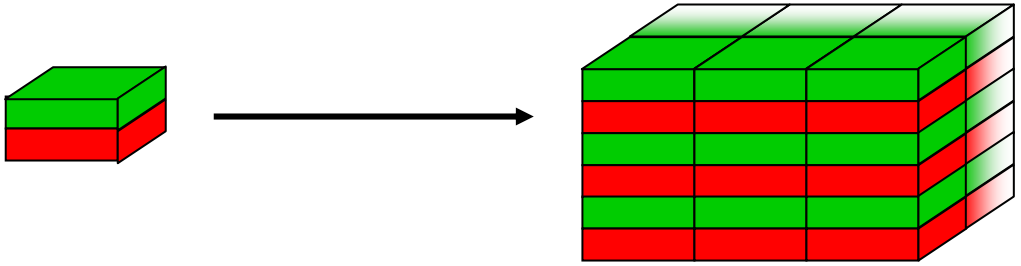
Modelling of interfaces

- Density functional theory → Hohenberg/Kohn/Sham, 60's

$$[-\tfrac{1}{2}\nabla^2 + v(r) + \int \frac{\rho(r')}{|r-r'|}dr' + v_{xc}(r)]\varphi_i(r) = \varepsilon_i\varphi_i(r)$$

E_{kin} E_{coul}^{n} E_{coul}^{e} E_{xc}

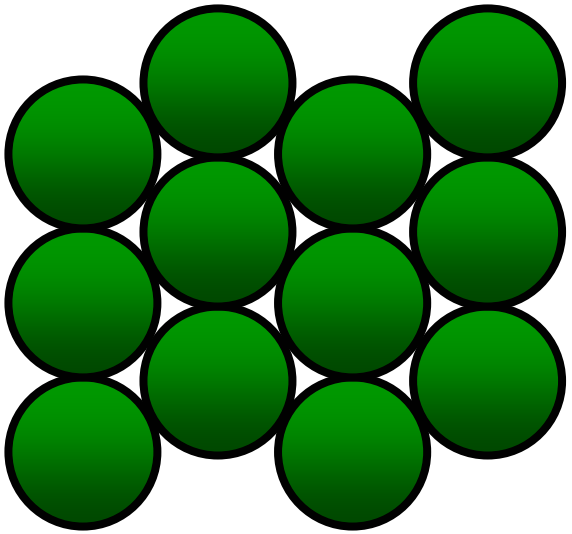
- Supercells - periodic boundary conditions



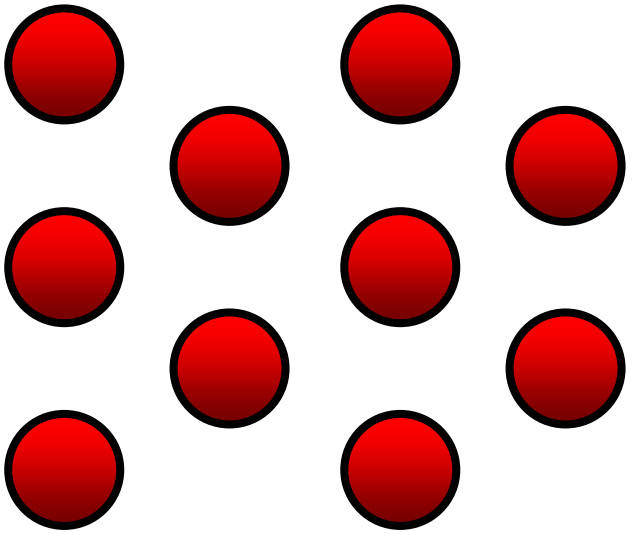
- Basis of plane waves for valence / semi-core
- Pseudopotentials for inner electrons + nucleus

Ti(0001) | Si(111) interface

Ti: hcp (0001)



Si: diamond (111)



ν = 26.8%

r(Ti) = 1.47

d(Ti-Ti) = 2.94

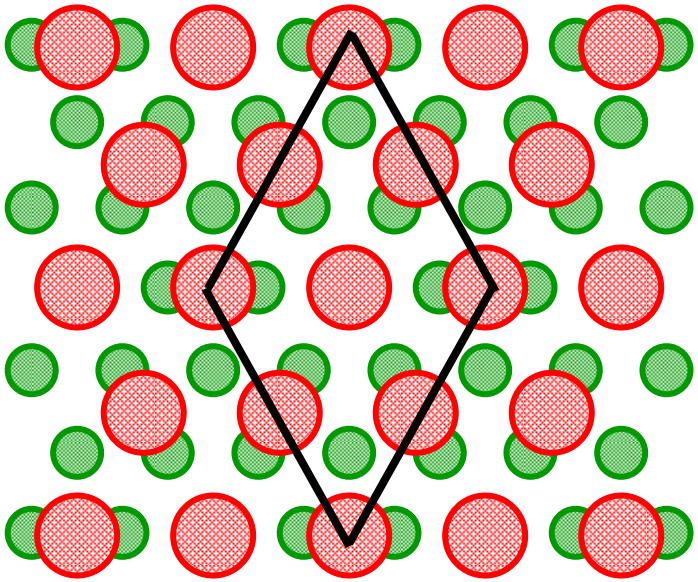
Silicides!

r(Si) = 1.11

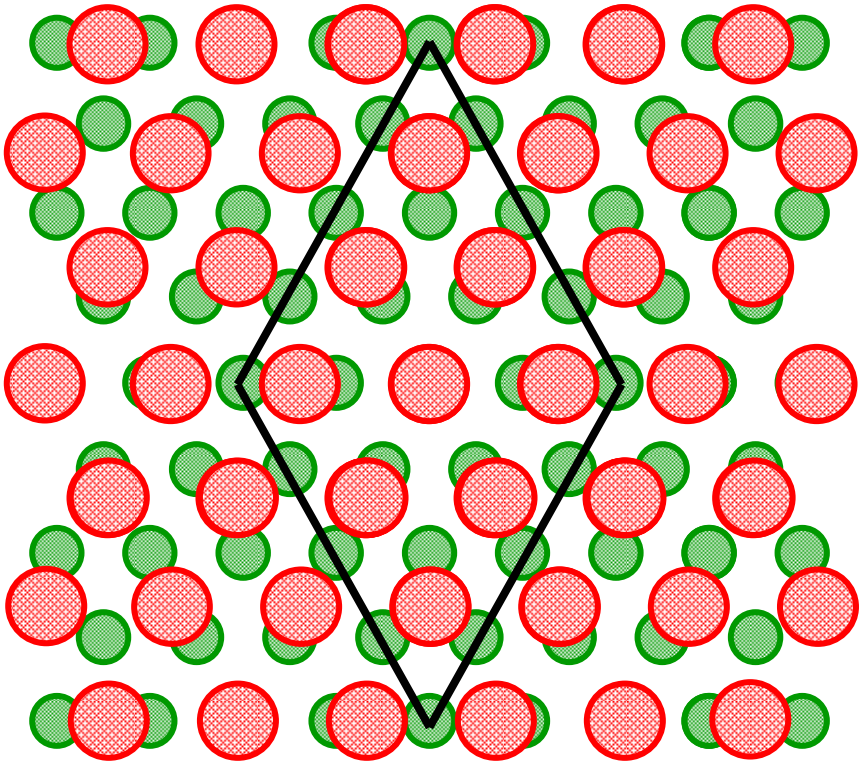
d(Si-Si) = 3.85

CSL for Ti(0001)|Si(111)

d(Ti) : d(Si) = 0.667



d(Ti) : d(Si) = 0.75 ≈ 0.76 (exp)



area density:

Ti : Si = 9 : 4 **(Ti_3Si)**

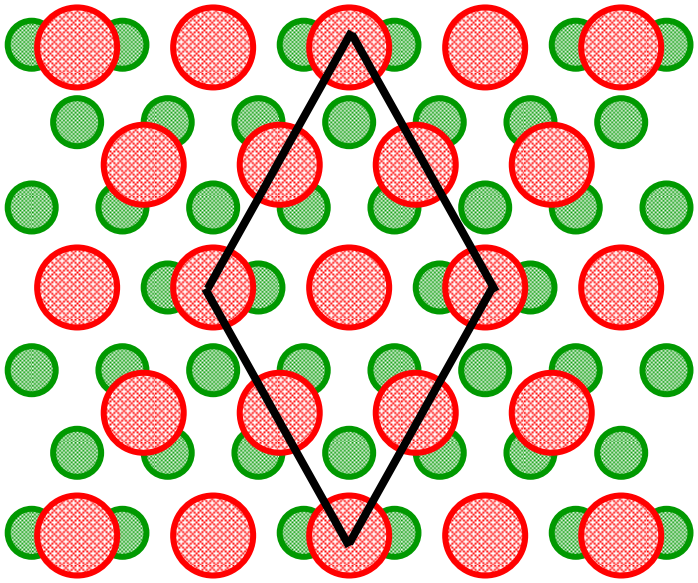
Ti : Si = 9 : 8 **(TiSi)**

Ti : Si = 16 : 9 **(Ti_2Si)**

Ti : Si = 16 : 18 **(TiSi)**

Binding strength – influence of mismatch

R = 0.667

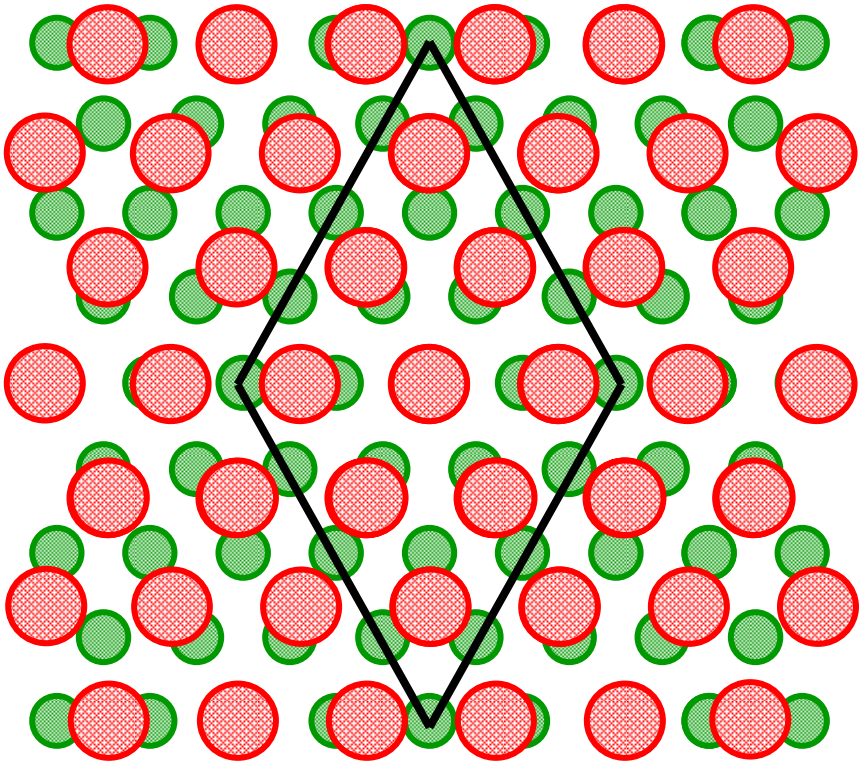


Exp.: R = 0.765

$\nu' = 13.6\%$

non-bonding

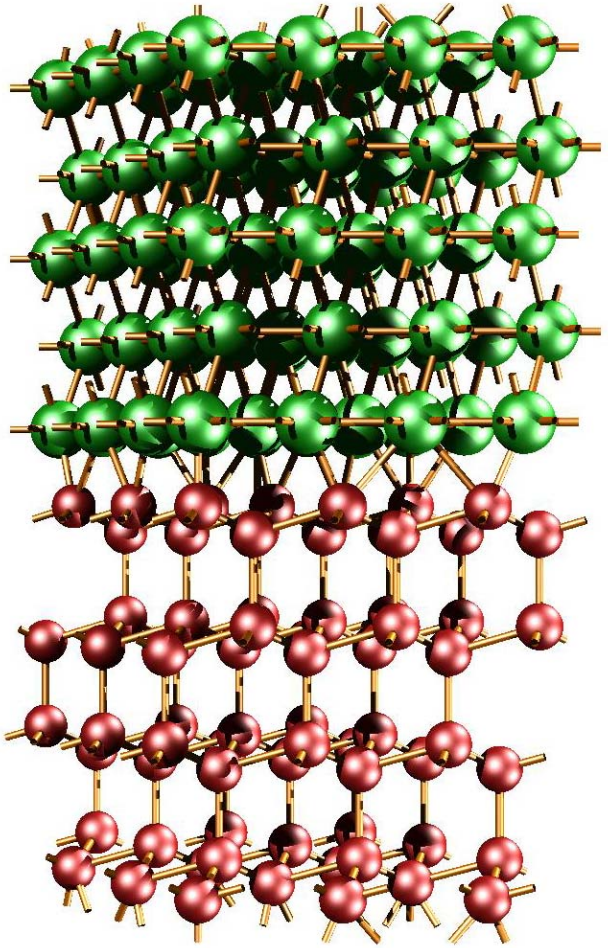
R = 0.75



$\nu' = 1.2\%$

W_{sep} = 0.28 J/m²

Supercell model

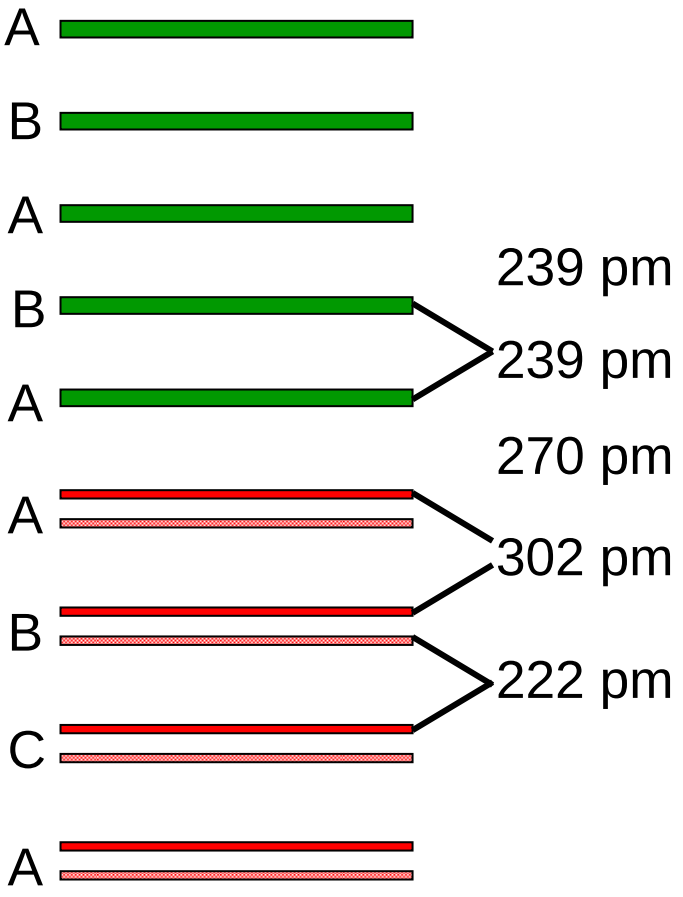


hcp

Ti(0001)

Si(111)

diamond



72 Si, 80 Ti

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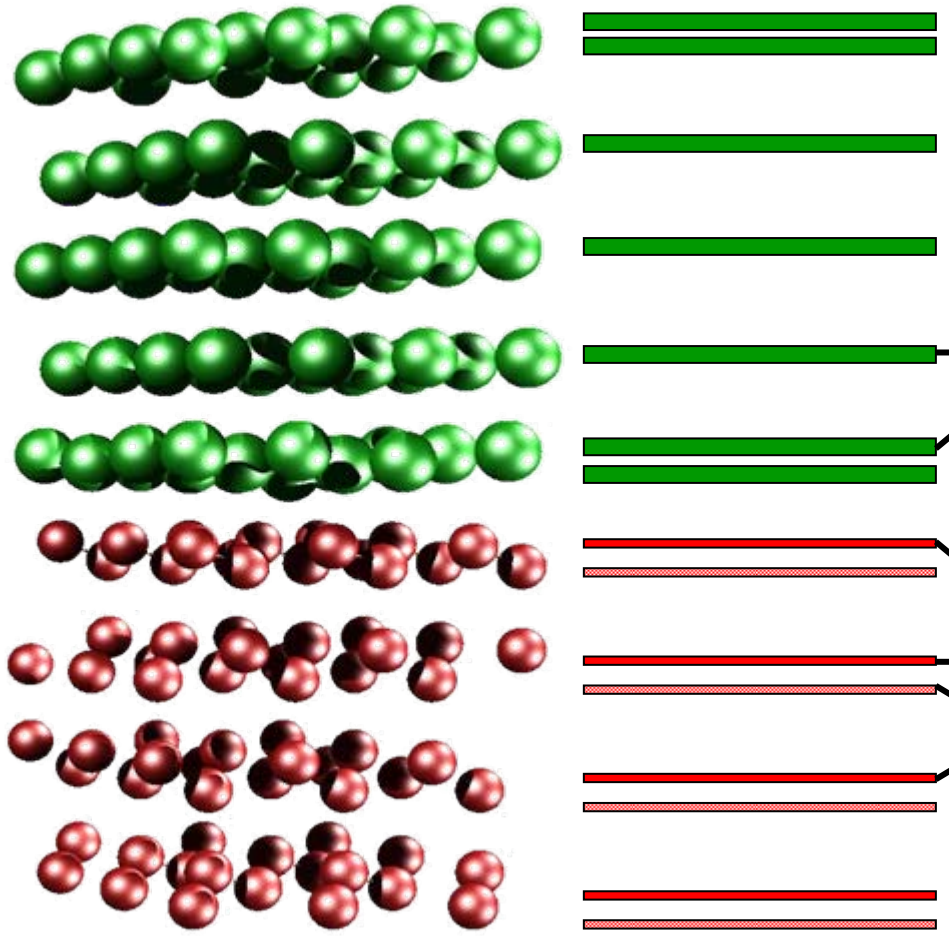
Institut für Ionenstrahlphysik
und Materialforschung

Static relaxation – weak bonding



239 pm
228 pm
9 pm
244 pm
58 pm
308 pm
222 pm
86 pm

enhanced rumpling

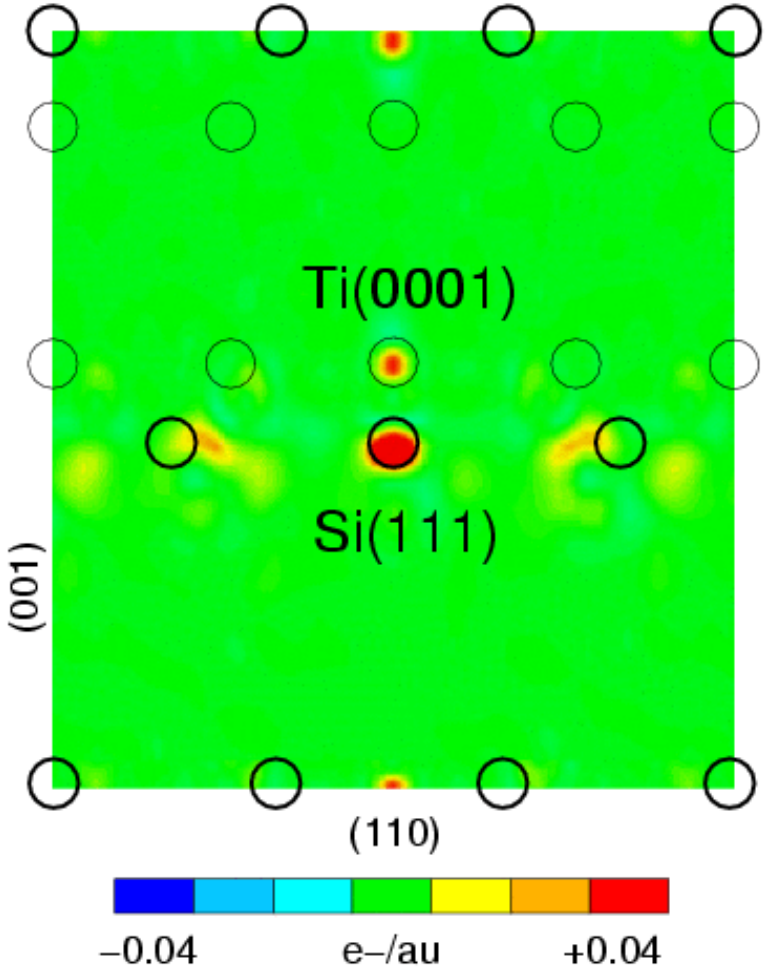
interface contraction

reduced rumpling

W_{sep} = 0.28 J/m²

T = (0,0,-0.26)

Bonding type – silicidation?



- Electron density difference:

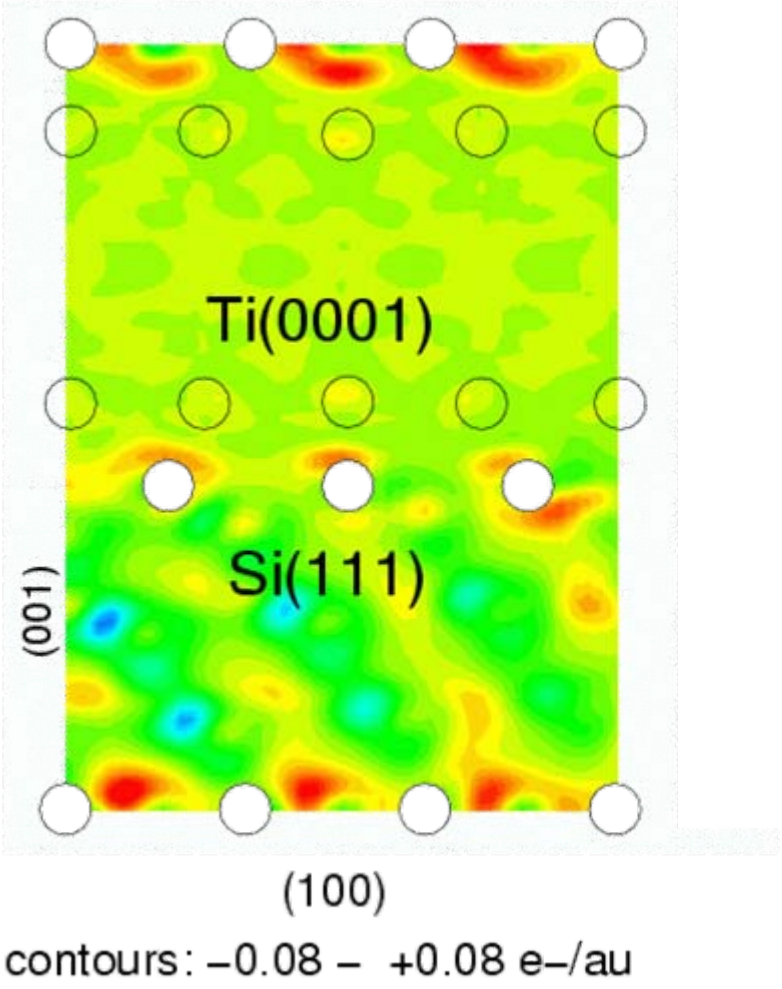
  $d\rho(\mathbf{r}) = \rho_{\mathbf{tot}} - \rho_{\mathbf{Si}} - \rho_{\mathbf{Ti}}$

- Minor redistribution of electron density upon Ti-Si-bonding

⇩

Weak interaction like noble metal|oxide

Bonding type – silicidation !



- Electron density difference:
  mainly at interface
- Major contributions
  electron enrichment at Si
  = indicator of silicide formation
  strong delocalisation at Ti

⇩

Not like noble metal|oxide
Reactive!

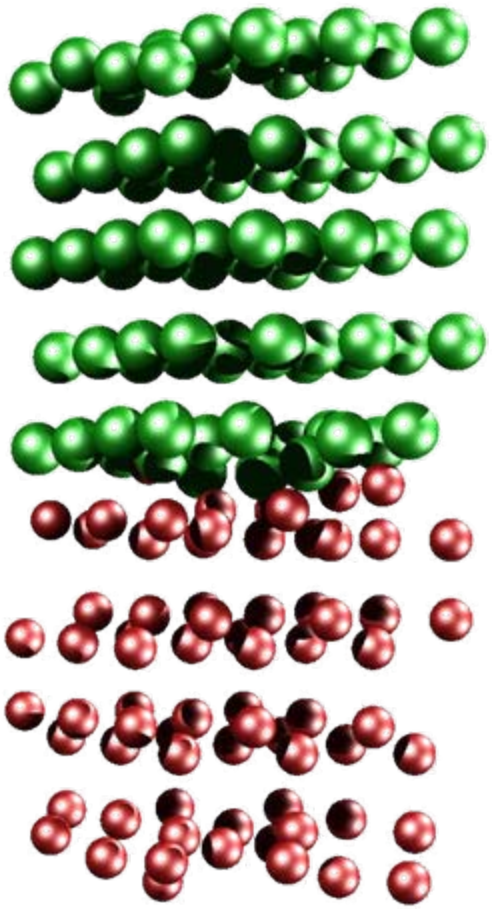
Atomistics + Electronics:

- ***only 10% "good" Ti-Si bonds***
- ***misfit important for W_{sep}***
- ***silicide formation***

What about the elastic part?

⇨ ***DFT-Molecular Dynamics (MD)***

Reacted interface at 300 K



metal

reaction zone

silicon

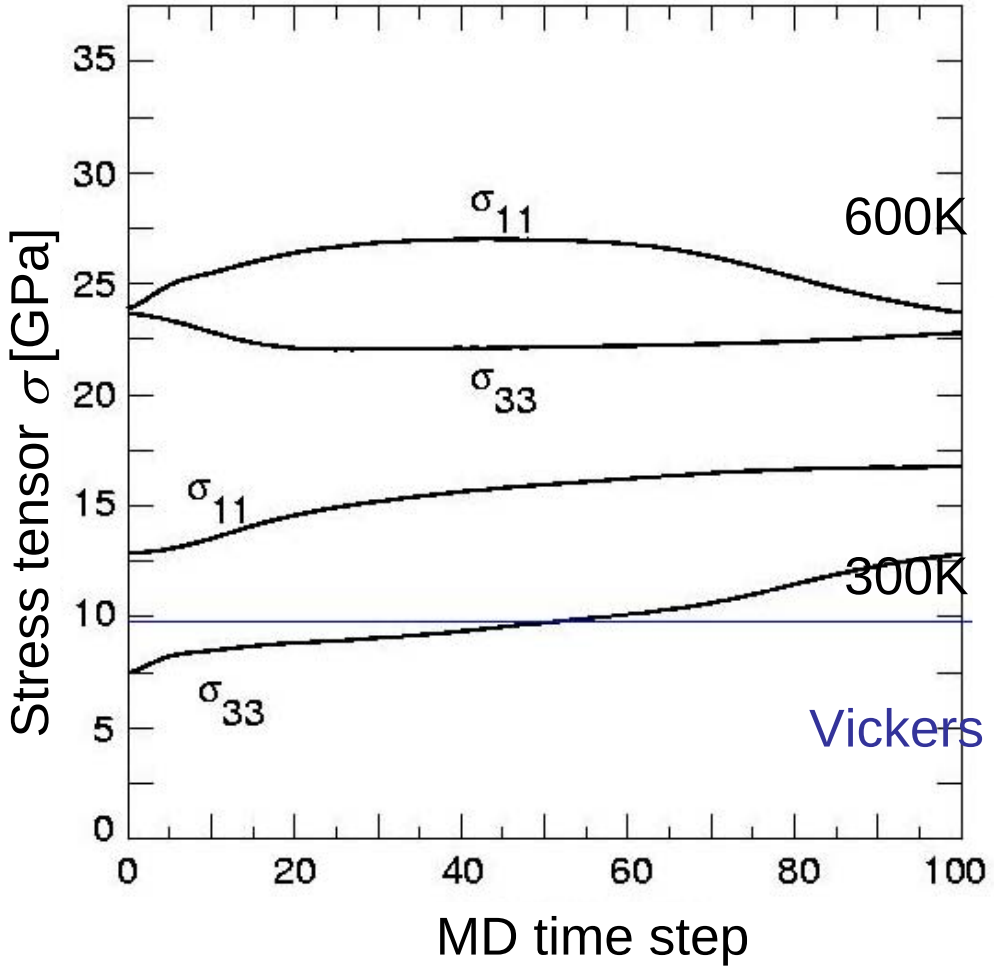
- Binary phase formation
- First full Si(111) layer
  + first Ti(0001) layer
- Stoichiometry Ti : Si = 1 : 1

⇩

$W_{sep} = 0.52\ J/m^2$

Further stabilisation!

Stres relaxation



- Reduction and equilibration of σ by binary compound formation

- $\sigma_{11} > \sigma_{33}$ lateral interaction > perp. direction

Silicide formation:

Electronic interactions **+** ***Elastic contributions***