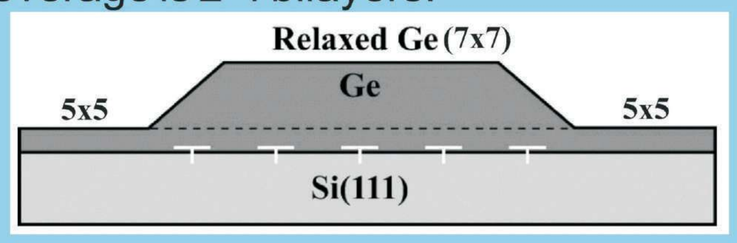
Si(111) strained layers structure on Ge(111) surface

R. Zhachuk,[1] J. Coutinho,[2] V. Cherepanov,[3,4] B. Voigtlander[3,4]
[1]Institute of Semiconductor Physics, pr. Lavrentyeva 13, Novosibirsk 630090, Russia
[2]I3N, University of Aveiro, Aveiro, Portugal
[3]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany

Experiment:
- Ge Islands as substrate: H = 150 Å, L = 5000 Å.
- T_{ads} = 400-550°C.
- Si coverage is 2-4 bilayers.

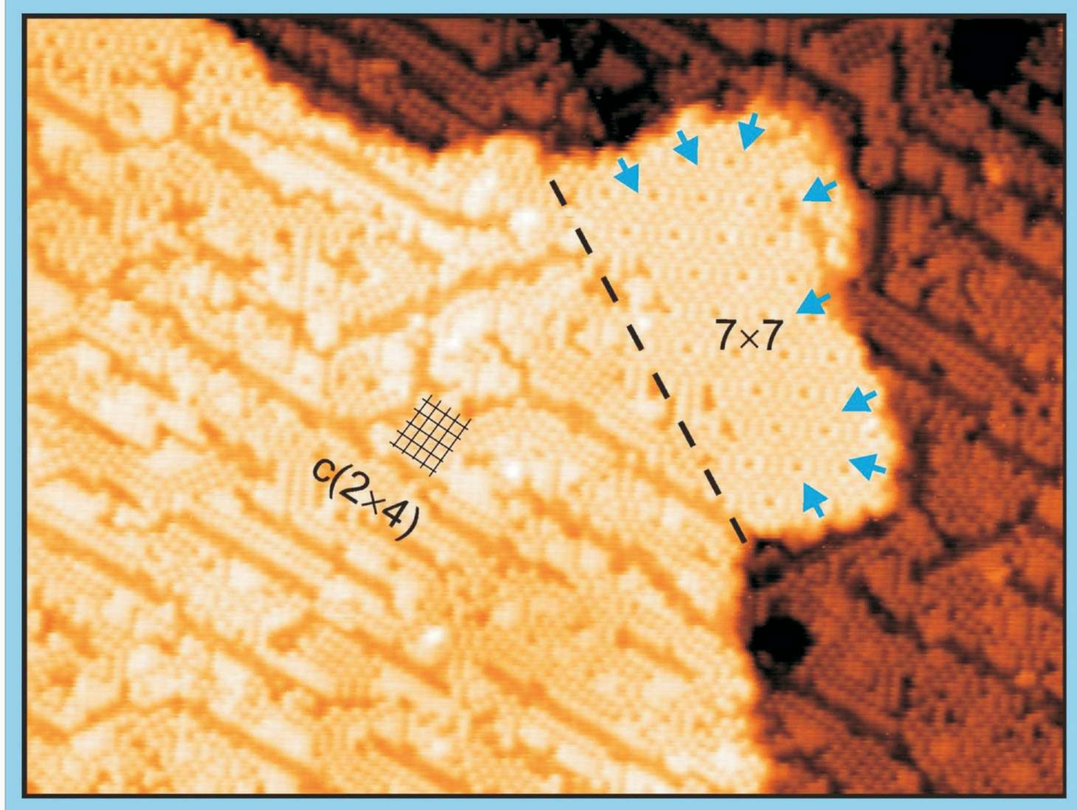


Motivation: calculations show that Si(111) and Ge(111) surface structure undergo the following transformation when surface strain is applied (from left to right: tensile strain, from right to left: compressive strain):

[DAS structures] ⟷ [adatom-based structures]

Aim: solve the atomic structure of tensile strained Si layers, formed during Si/Ge(111) growth. **Methods:** LEED, STM (Omicron), DFT (Siesta).

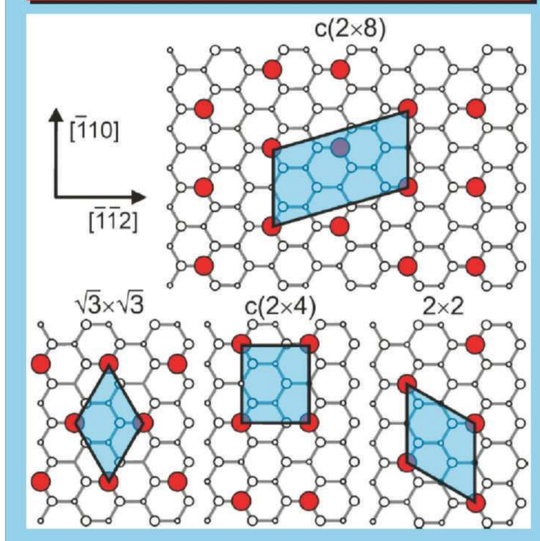
STM image of the Si/Ge(111) surface



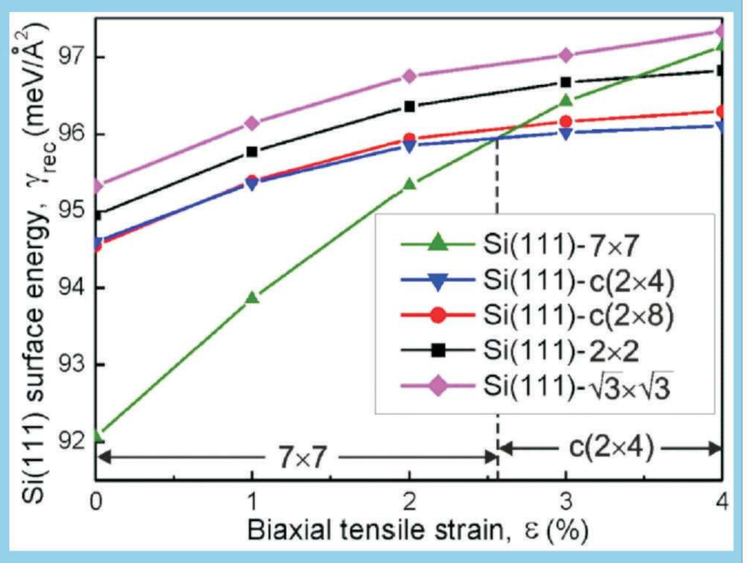
2 bilayers of Si on Ge(111), T_{ads}=540 C

1. No Ge/Si intermixing

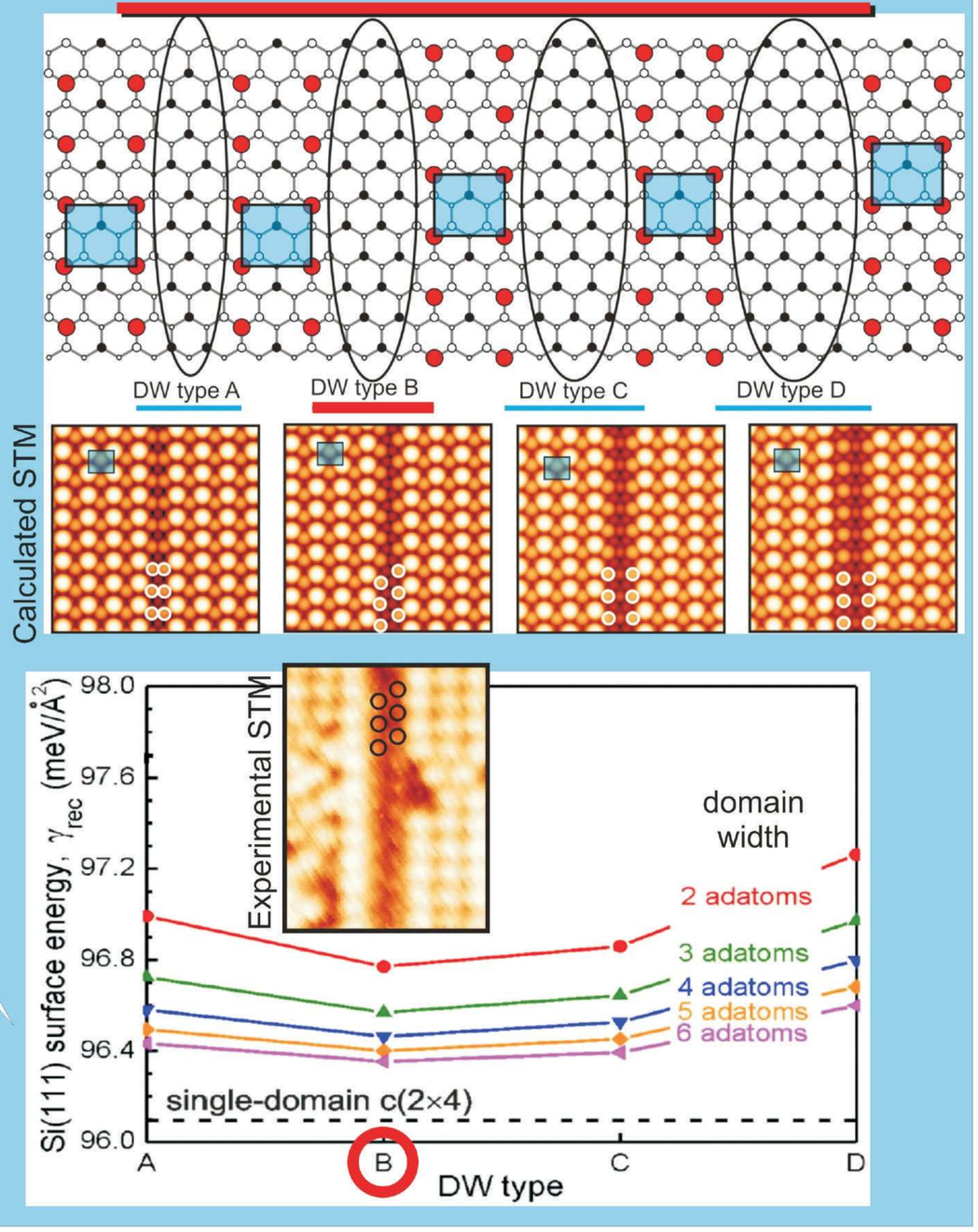
Adatom-based structures



Si(111) phase diagram

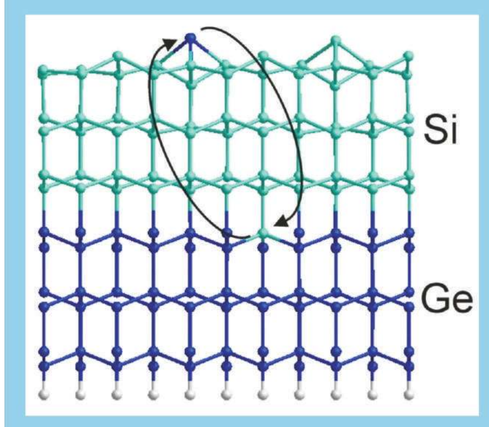


Atomic structure of domain walls (DW)



Domain walls do not form when no Ge and Si intermixing is considered, since they do not lead to relaxation of Si layers!

2. Ge/Si intermixing



Surface structure	Surface energy (meV/A^2)	
	no intermixing	intermixing
c(2x4)	96.1	82.9
c(2x4) + DW	96.6	82.4

(DW type "B", width is 3 adatoms)

- Si and Ge atoms are undistinguishable in STM.
- Energy gain is 0.4 eV per Si-Ge pair when Ge substitutes Si atom with dangling bond (adatoms or rest-atoms). This energy gain is due to Si bonds being stronger than that of Ge.
- Density of dangling bonds in DW is twice higher than in c(2x4) structure.
- DW is energetically favorable when Si/Ge intermixing is considered. Ge local concentration in DW must be higher that that in the c(2x4) structure (i.e. nanowires).

Conclusions:
1) Under tensile strain the Si(111) surface structure changes 7x7 (DAS) → c(2x4) (adatom-based) in agreement with calculations.
2) Atomic models of the c(2x4) structure and its domain walls are developed.
3) The reason for c(2x4) domain walls formation is intermixing of Ge and Si atoms.