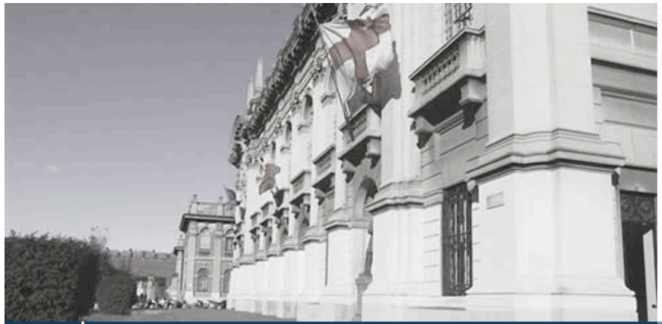

POLITECNICO DI MILANO

Ge/SiGe Superlattices for Thermoelectric Applications

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Outline

- Thermoelectric (TE) Effect
  - Possible Applications
  - Figure of Merit
  - p-type Thermoelectric Materials
- Figure of Merit Improvement
- Lateral p-type Ge/SiGe Superlattice TE Design
  - Active Layer Requirements
- Low-Energy Plasma-Enhanced CVD (LEPECVD)
- XRD and TEM Superlattices Characterization
- Lateral TE Device: Fabrication Features
- Thermal Conductivity Reduction: Phonon Engineering
- Conclusions

Thermoelectric Effect

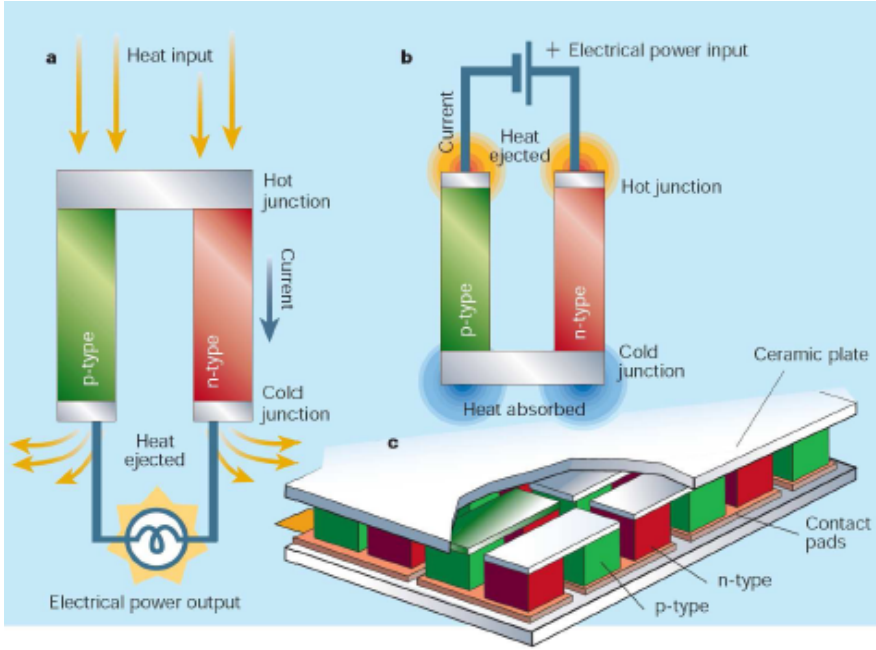
Power Generation:

$\Delta T \rightarrow \Delta V$ (Seebeck effect)

Cooling and Heating Elements:

$\Delta V \rightarrow \Delta T$ (Peltier effect)

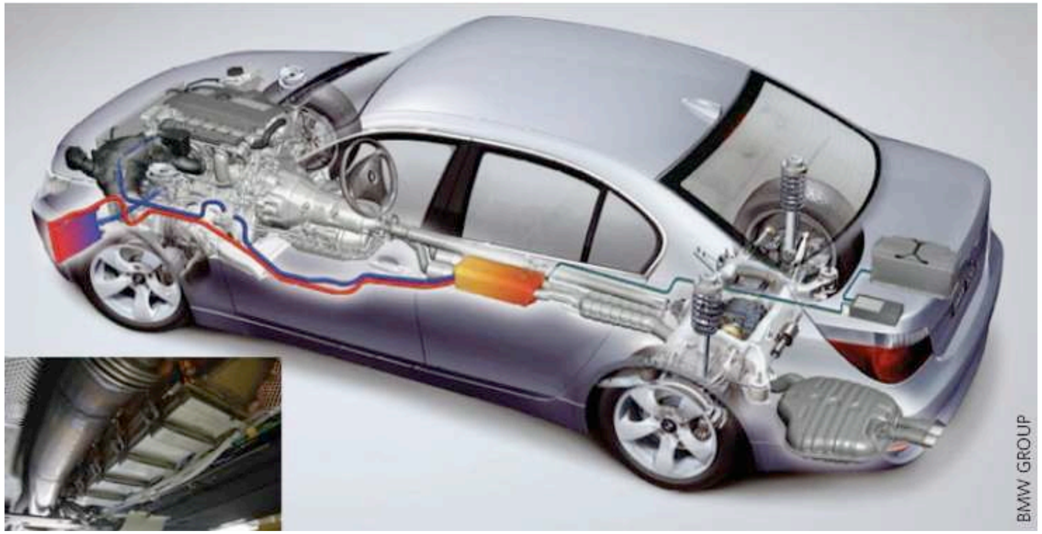
An applied temperature gradient causes charged carriers in the material to diffuse from the hot side to the cold side, similar to a classical gas that expands when heated

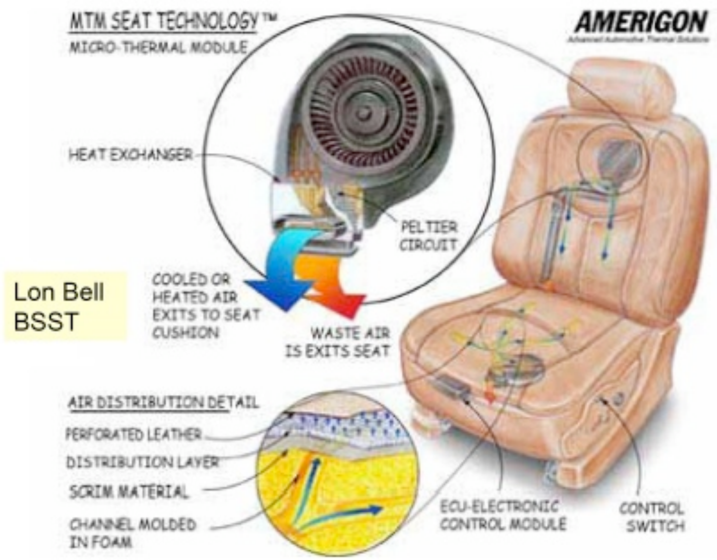


$\Delta T > 5°C$

Possible applications of TE

- Integrated on-chip energy harvesting
- Power autonomous systems such as human body sensors
- Automobile waste-heat recovery
- Wrist-watches (Seiko Thermic)
- Combined heat and power system (CHP)
- Peltier coolers





Efficiency of a Thermoelectric Material: The Figure of Merit *ZT*

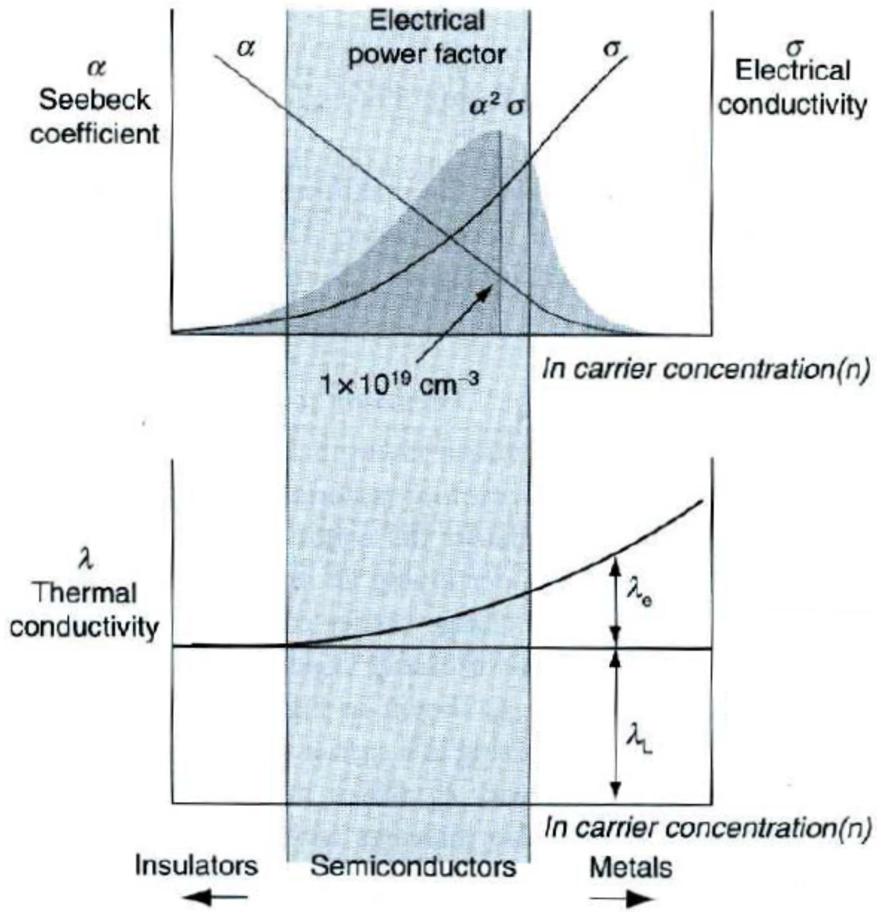
$$ZT = \frac{\alpha^2 \sigma}{\lambda} T$$

- α = Seebeck coefficient = $\frac{\Delta V}{\Delta T}$
- T = Absolute temperature
- σ = Electrical coductivity
- $\lambda = \lambda_{lattice} + \lambda_{electronic}$ = Thermal conductivity

→ Maximize $\alpha^2\sigma$

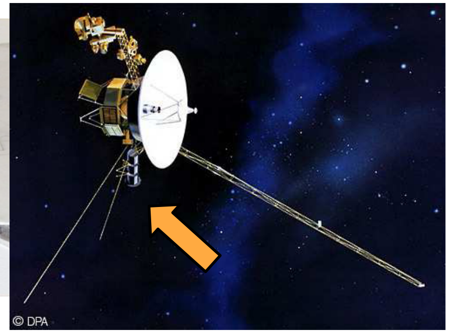
→ High electrical conductivity combined with low thermal conductivity

→ Wiedemann-Franz law: $\frac{\lambda_e}{\sigma} \propto T$



p-type Thermoelectric Materials

- **Bi_2Te_3**
  - Rare materials
  - Difficult to integrate onto silicon chips
- **Si and SiGe**
  - Compatible with backend CMOS and MEMS processing
  - Best performances for high temperature (above 500°C)
  - Most prominent application: radioisotope thermoelectric generators (RTG) in deep space applications (e.g. Voyager 1&2, Cassini, …)

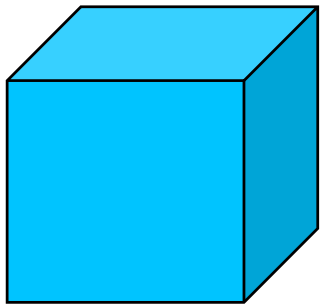


[http://www.jpl.nasa.gov

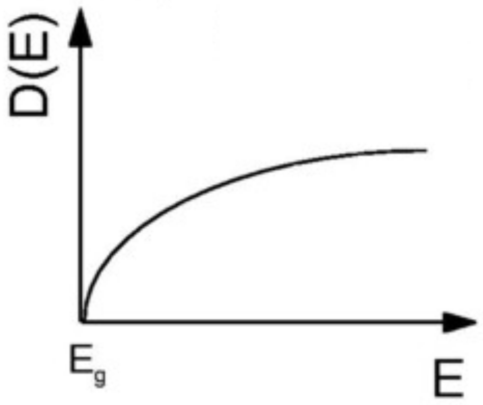
Material at 300 K	N [cm^{-3}]	ρ [Ωm]	α [μVK^{-1}]	κ [$Wm^{-1}K^{-1}$]	ZT (300K)
$(BiSb)_2 Te_3$	–	1.2×10^{-5}	175	2.0	0.375
Si	1.5×10^{19}	9.0×10^{-5}	148	148	0.00049
Ge	1.0×10^{19}	2.8×10^{-5}	280	59.9	0.014
$Si_{0.72}Ge_{0.28}$	3.4×10^{19}	4.0×10^{-5}	245	6.5	0.069

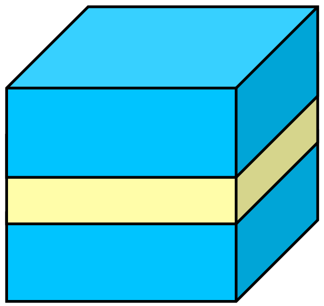
Stefano Carlo Cecchi - stefanocarlocecchi@gmail.com

Increase the TE figure of merit using superlattices (SL) structures

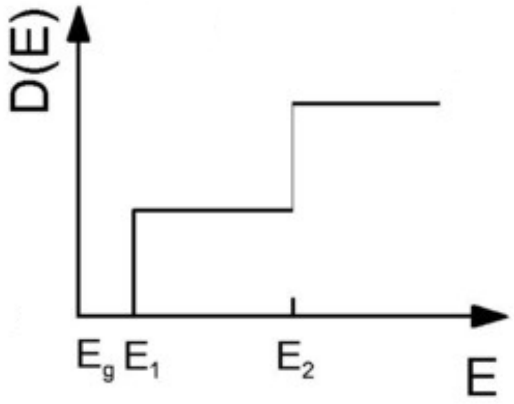


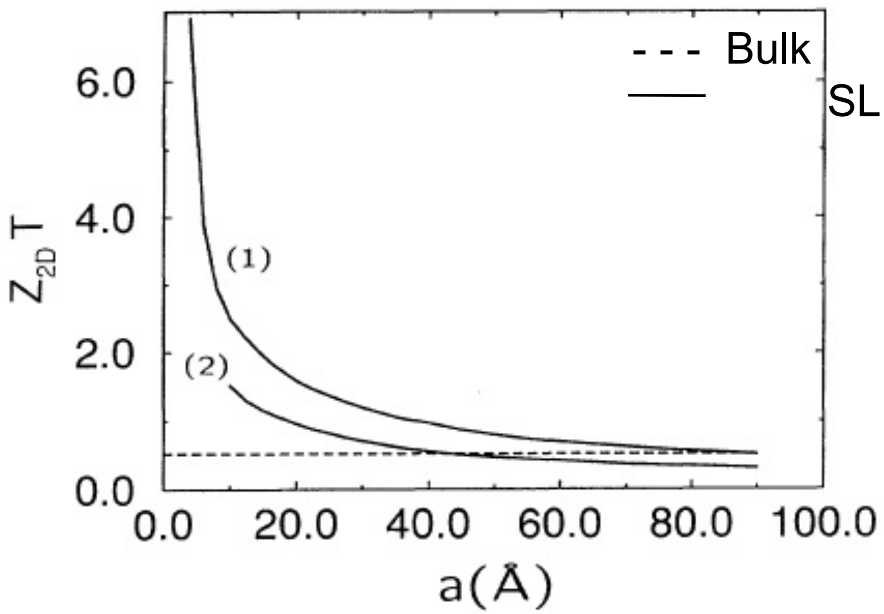
Bulk
(3D structure)





Quantum Well
(2D structure)



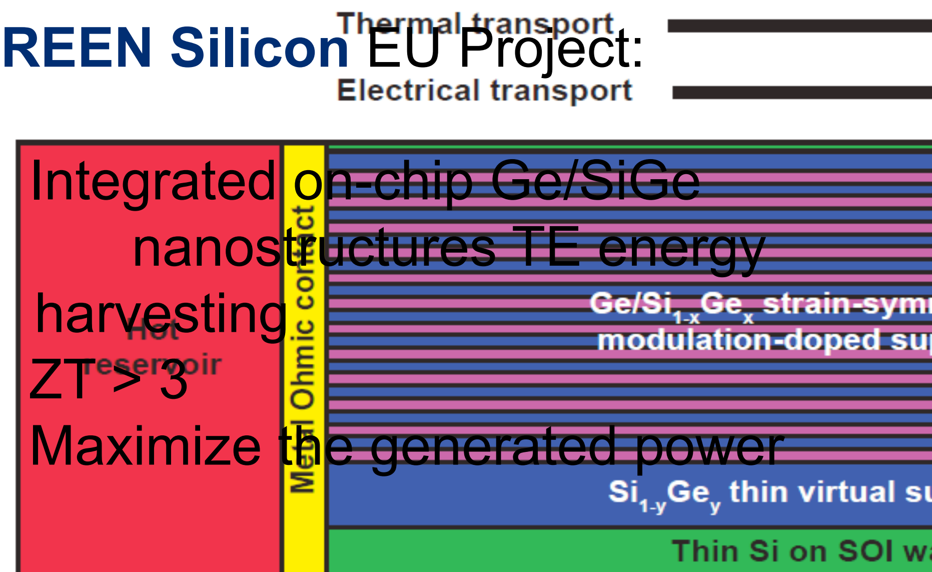


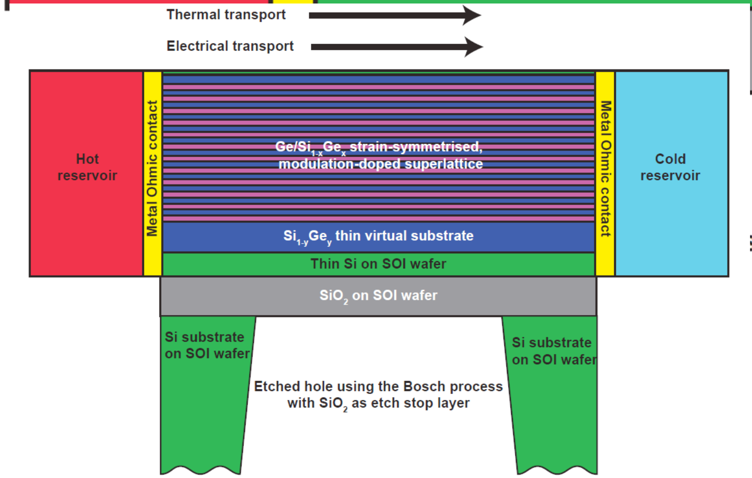
[L. D. Hicks, M. S. Dresselhaus, Phys. Rev. B 47, 12727 - 12731 (1993)]

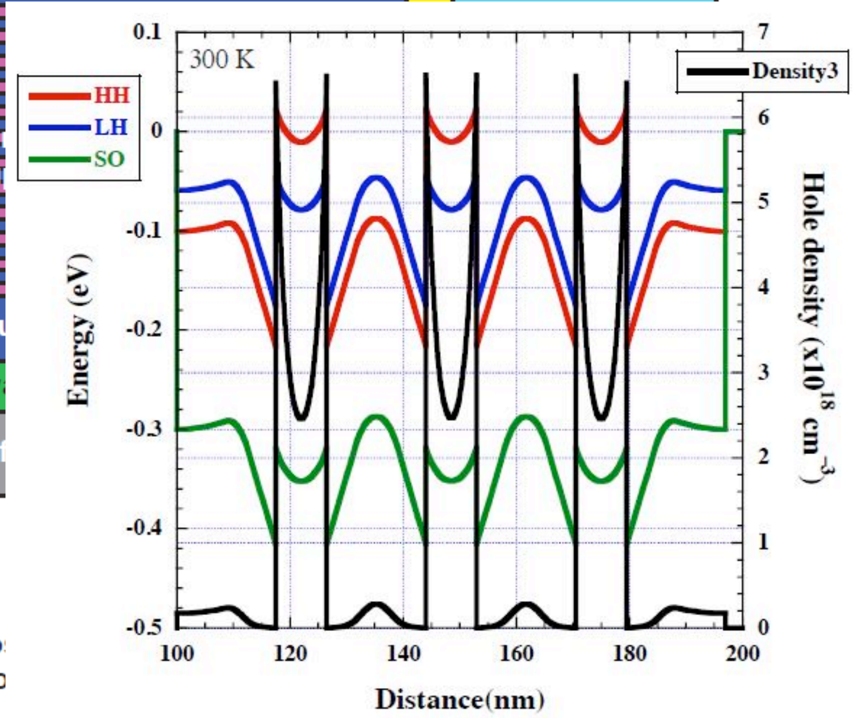
Lateral p-type Ge/SiGe Superlattice Thermoelectric Design

GREEN Silicon EU Project:

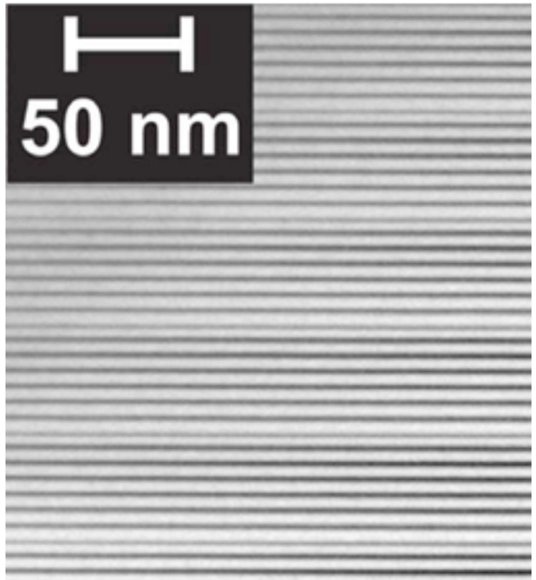
- Integrated on-chip Ge/SiGe nanostructures TE energy harvesting
- ZT > 3
- Maximize the generated power







Active Layer Requirements



- Maximize the generated power: $P \propto N_P$

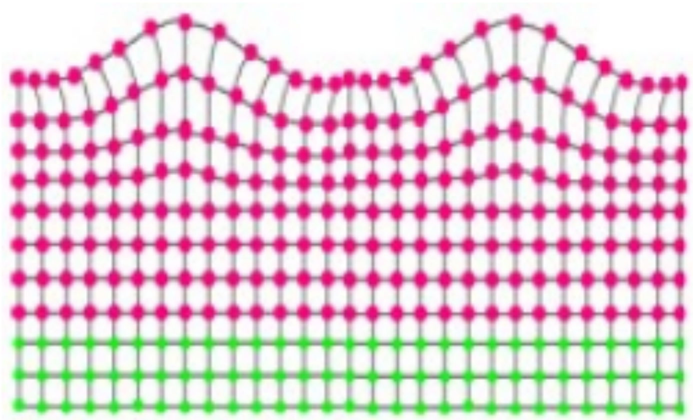
  → **~10 µm Ge/$Si_{1-x}Ge_x$ strain-symmetrised superlattice structure**

- Increase the thicknesses ratio $\dfrac{t_{active}}{t_{substrate}}$

  → **SOI substrates**

- Not trivial design for SiGe structures

  → **high-quality interfaces**
  → **thicknesses control**
  → **strain-symmetrised structures**



→ **LEPECVD**

Low Energy Plasma Enhanced Chemical Vapor Deposition (LEPECVD) - Basics

Gas-source plasma-assisted process

→ no thermal energy contribution

→ limited effect of surface chemistry

↓

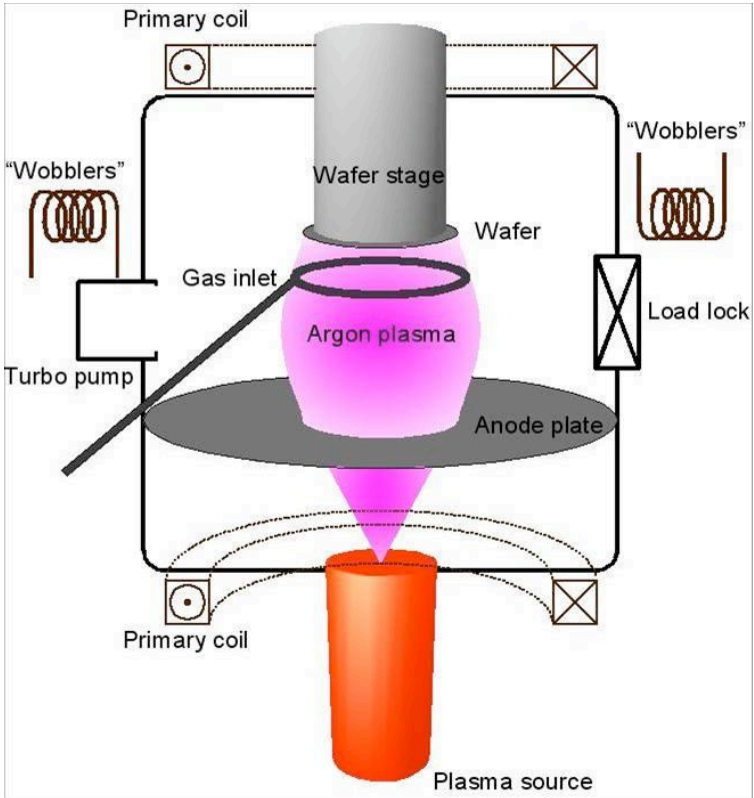
Film composition and growth rate are independent from substrate temperature

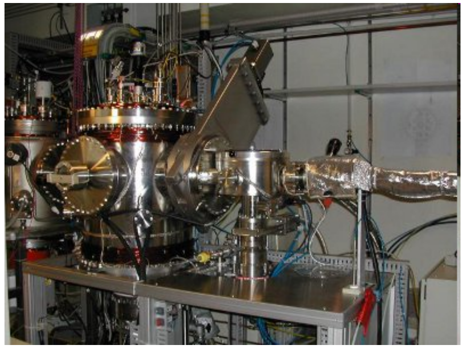
High density - low energy plasma

no ion-induced damage → epitaxy

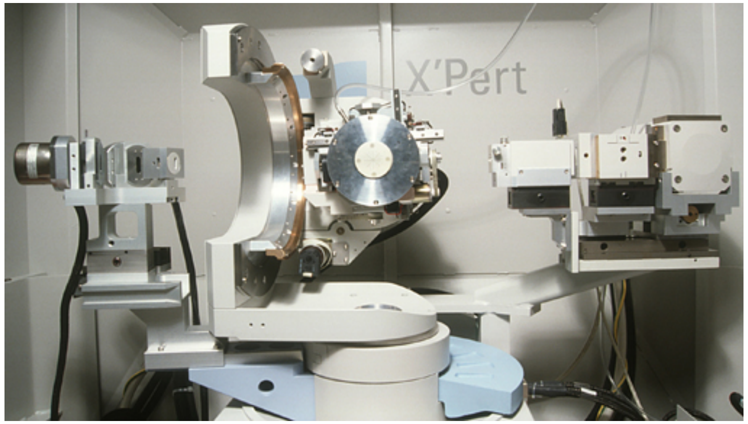
Wide range of growth rates

(0.1 Å/s to 10 nm/s)

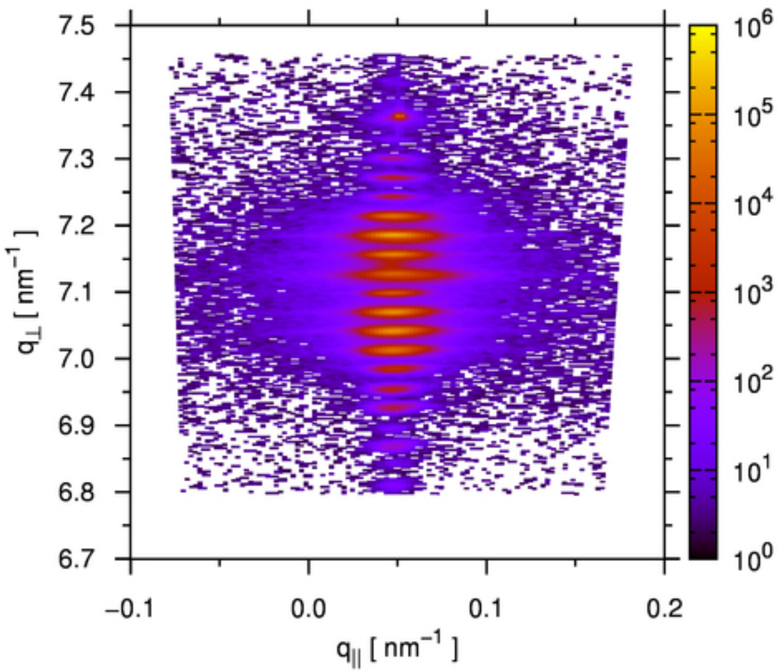




HR-XRD: Structural Characterization of SiGe Heterostructures [1]

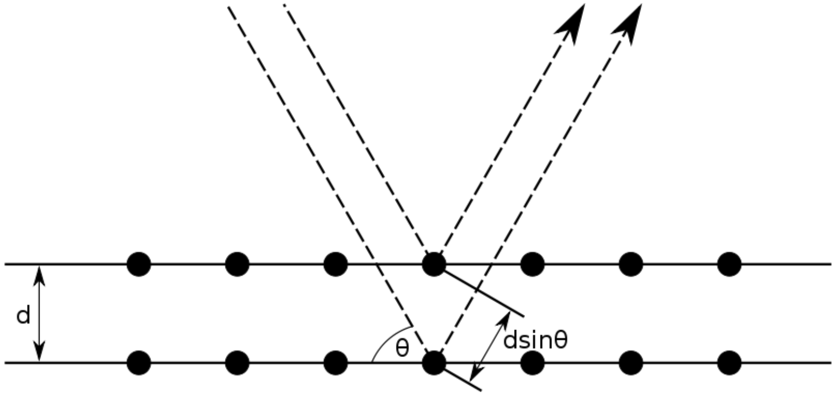


- Alloy composition
- Film relaxation
- Material and structures quality
  - Crystal quality (peaks intensity)
  - Interface quality (# of peaks)
  - Period (fringes period)



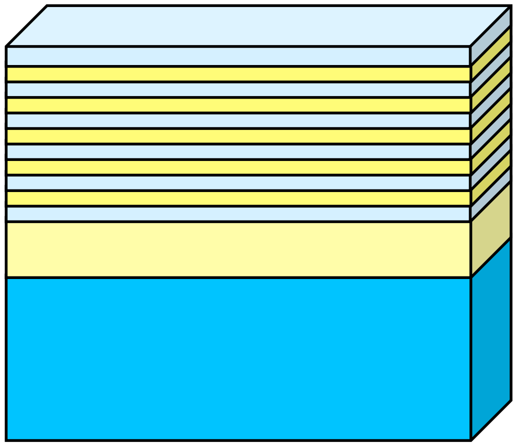
Complete characterization of SiGe heterostructures

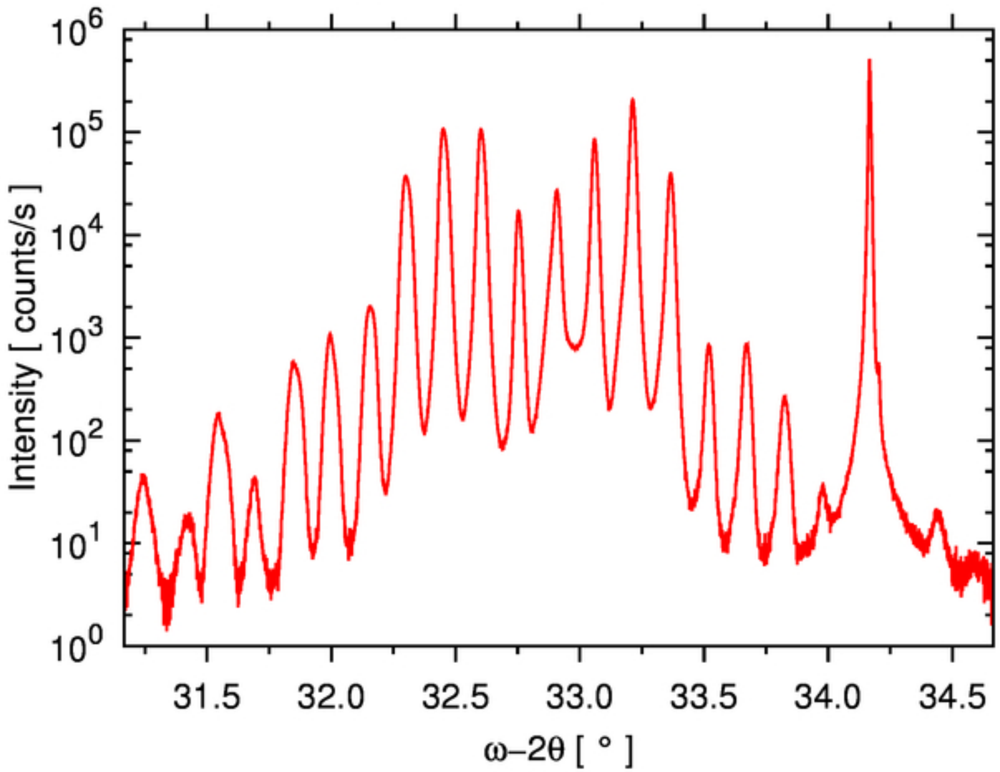
HR-XRD: Structural Characterization of SiGe Heterostructures [2]



Bragg Condition

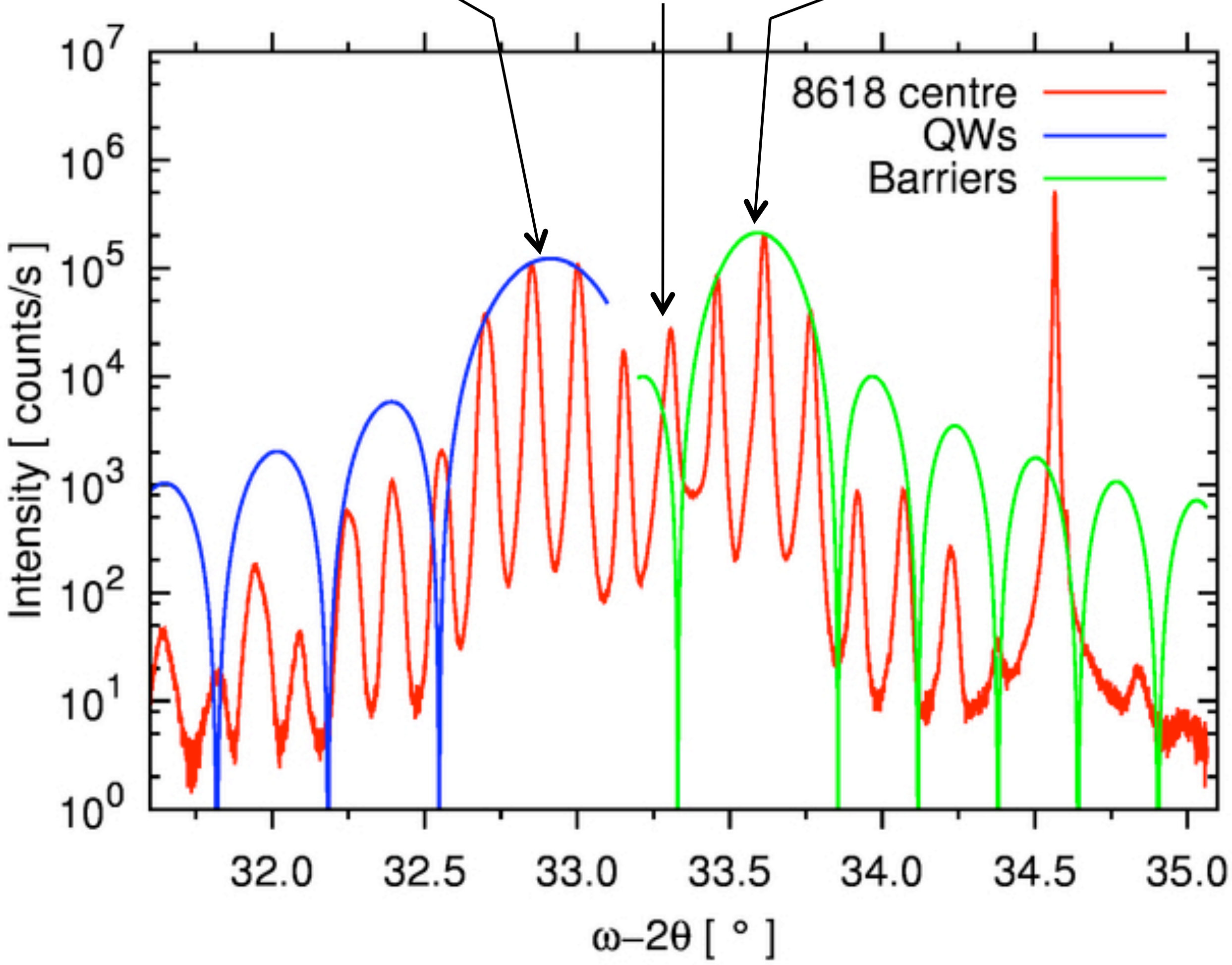
$$2d \sin\theta = n\lambda$$





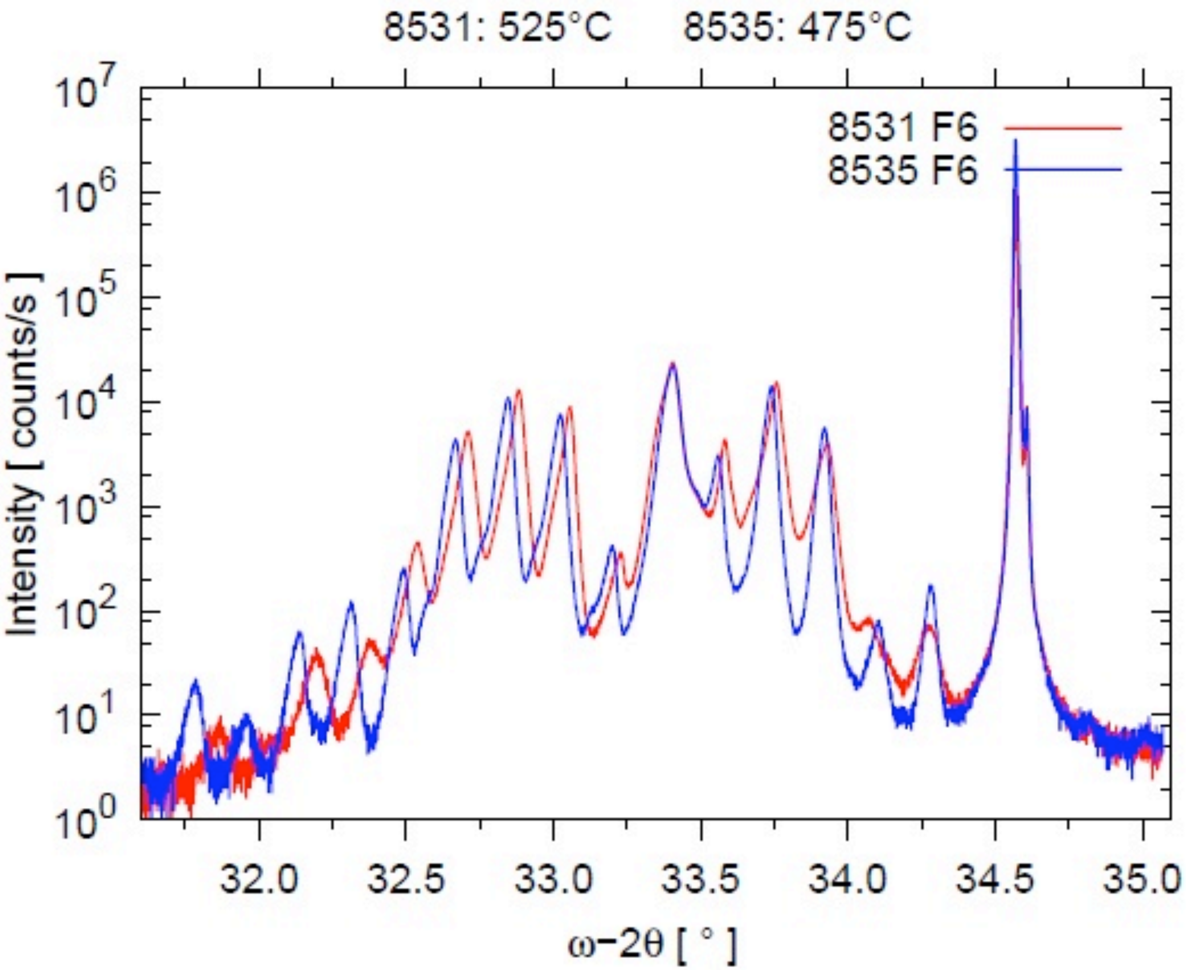
HR-XRD: Structural Characterization of SiGe Heterostructures [3]

X_{well} = 97,02% X_{0_peak} = 82,9% $X_{barrier}$ = 72,45%



T_{well} = 14 nm P_{SL} = 34,97 nm $T_{barrier}$ = 19,54 nm

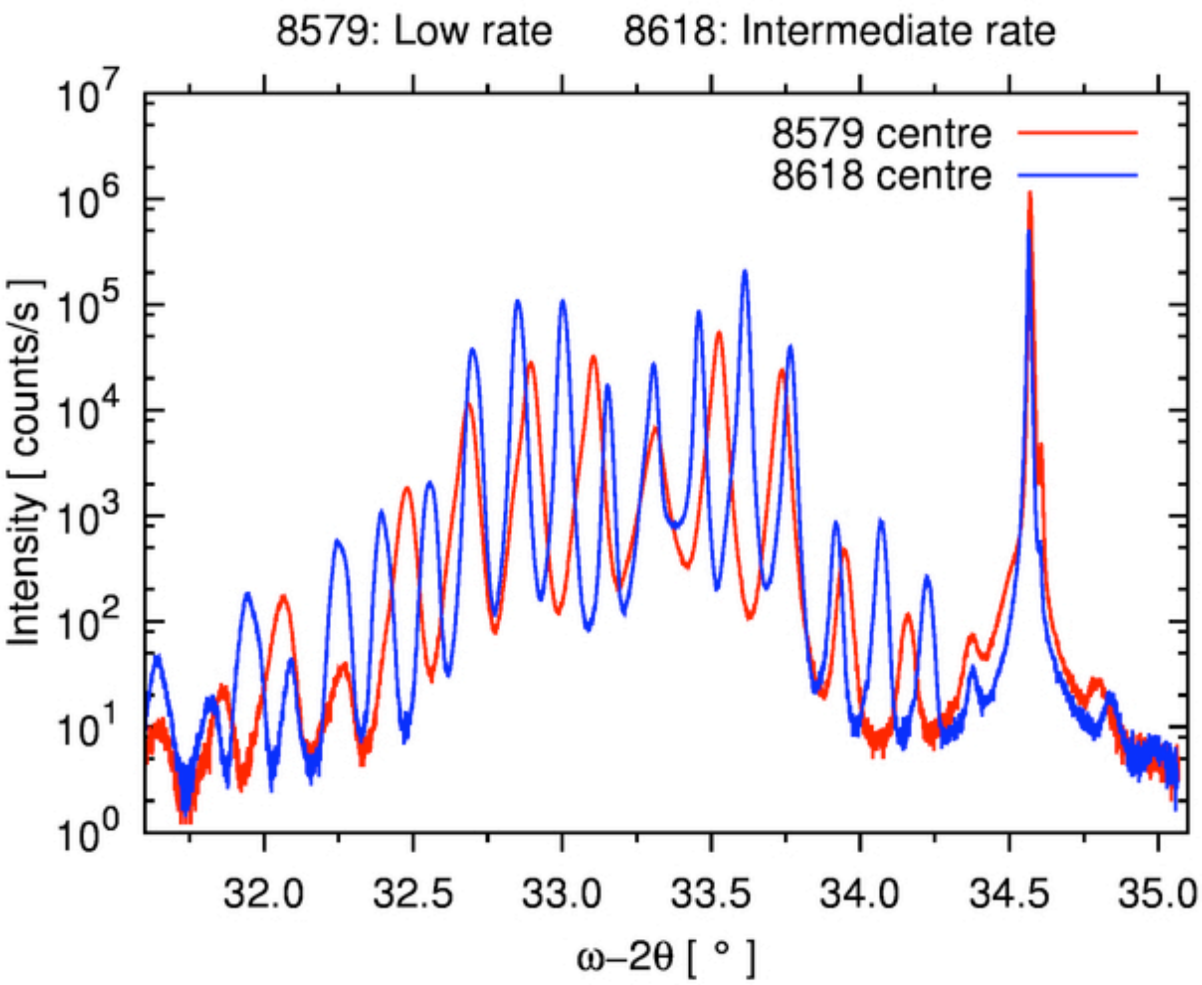
HR-XRD Characterization: Structure Quality vs Temperature



High intensity peaks in the regions around 32.0°and 34.25°for 8535 (grown at lower temperature)

better heterointerfaces due to reduction of interdiffusion and roughening

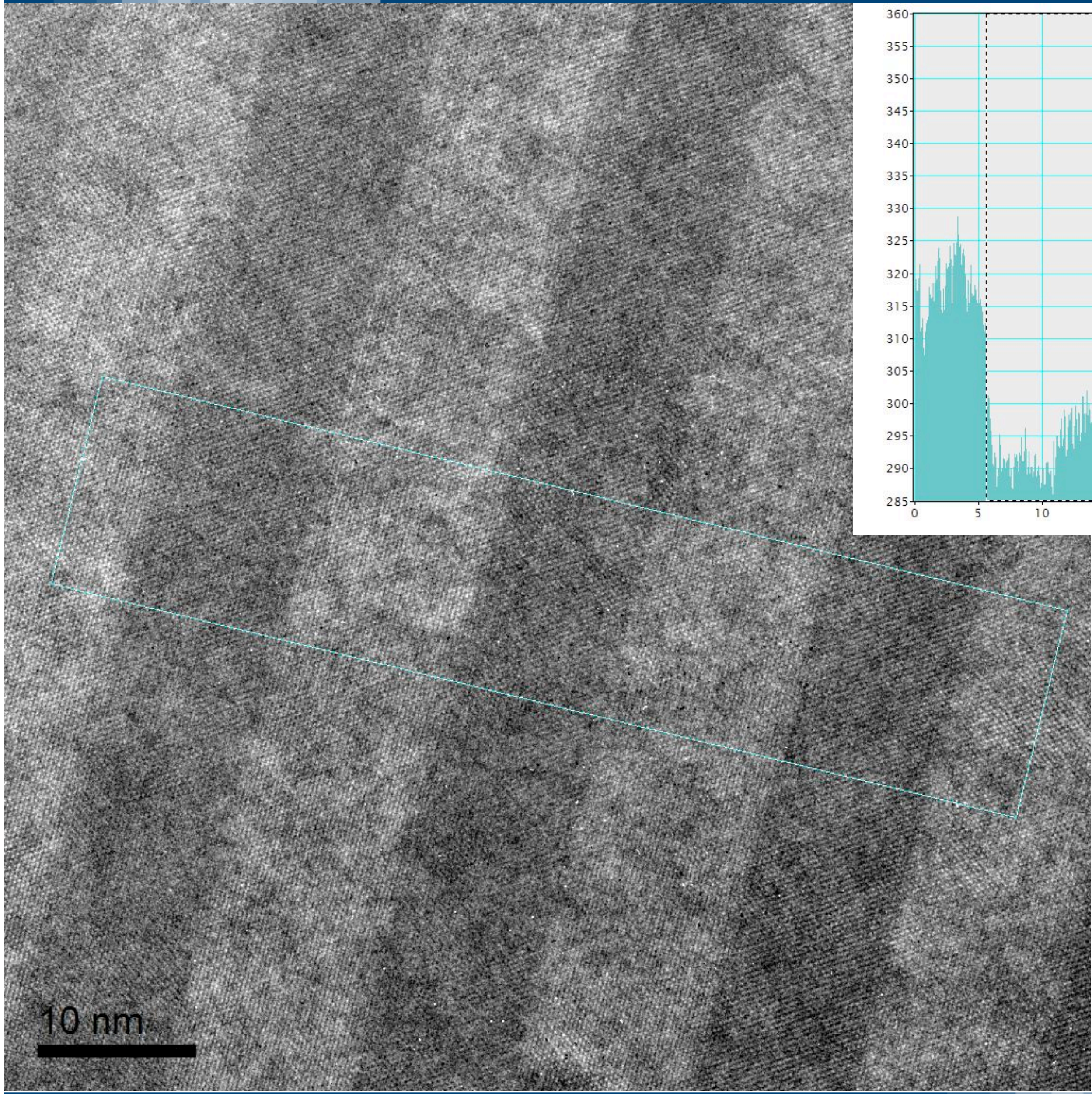
HR-XRD Characterization: Structure Quality vs Deposition Rate

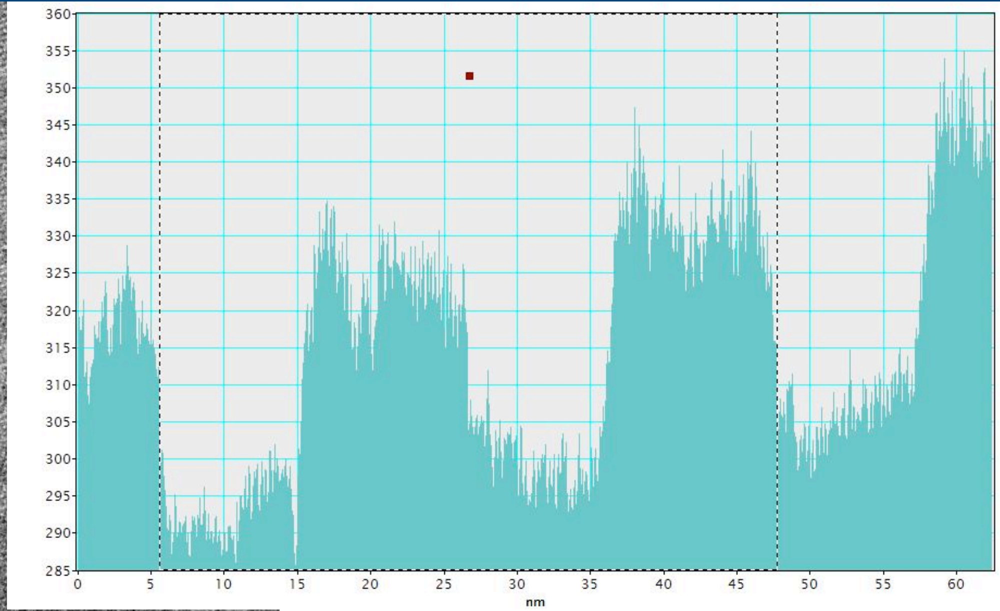


High intensity peaks in the entire region for 8618 (grown at ~1 nm/s, 4 times higher rate than 8579)

better heterointerfaces due to reduction of interdiffusion

HRTEM Investigation



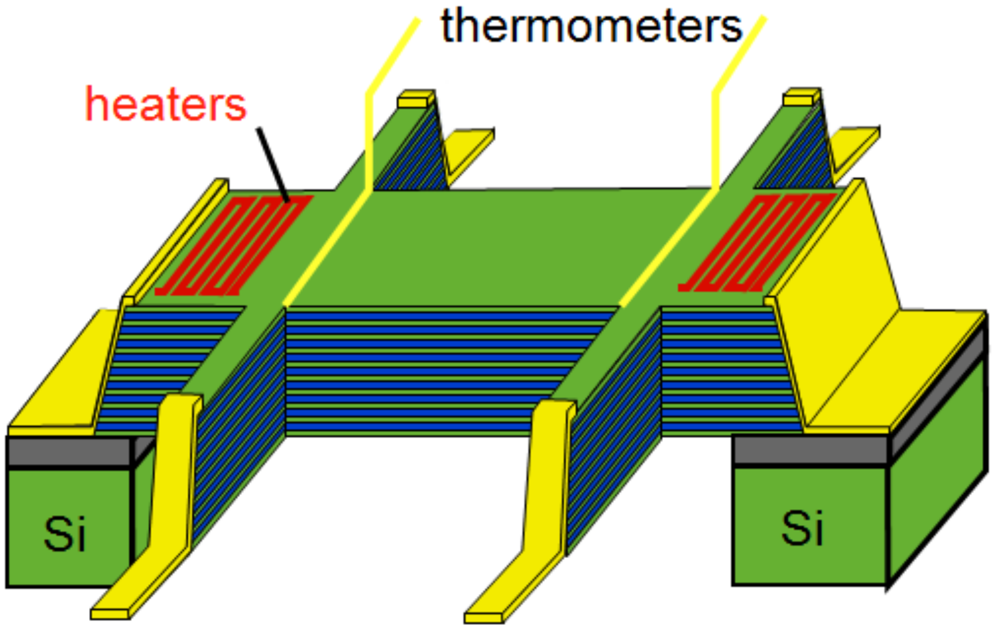


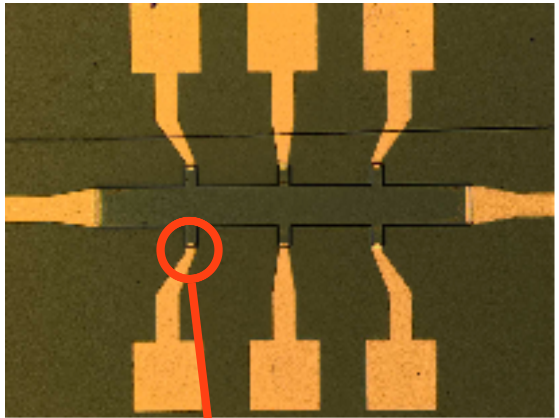
Profile Of HRTEM top layers

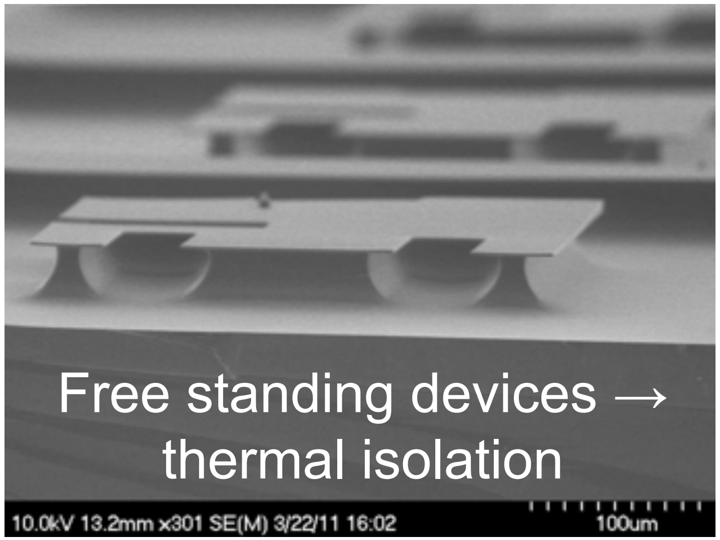
Determination of layer thicknesses

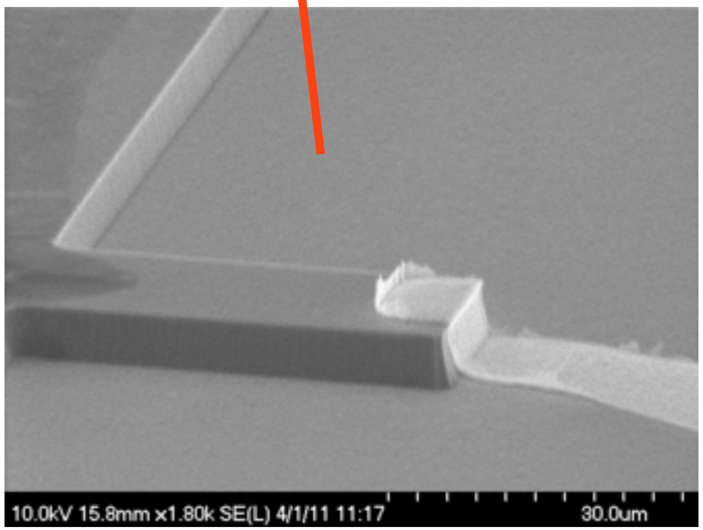
Intensity profiles along the growth direction (being averaged parallel to the interfaces over 200 pixels) were used. The faint blue frame in the HRTEM image indicates from which the intensity profile was taken.

Lateral TE Device: Fabrication Features



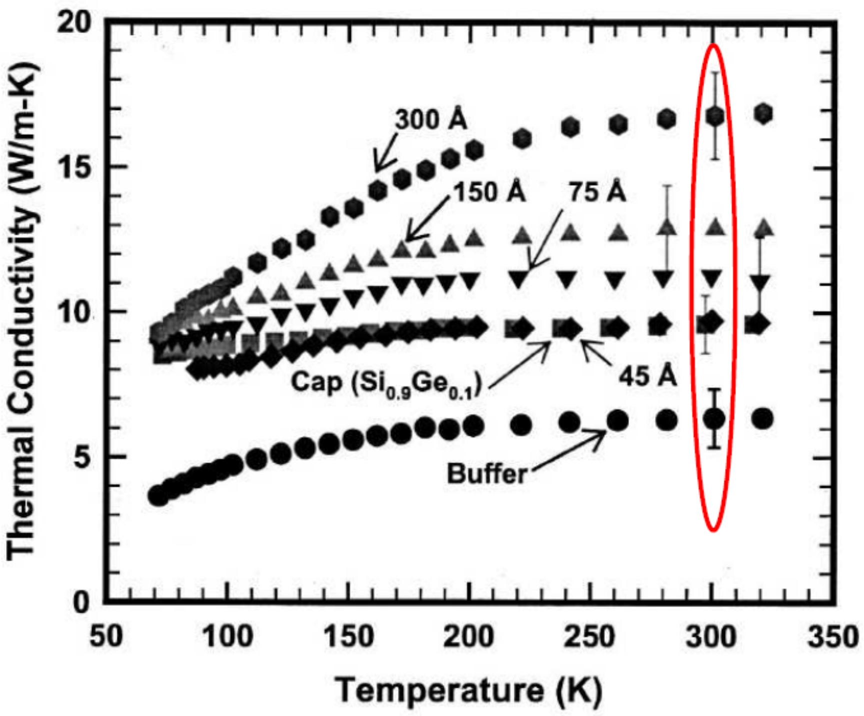


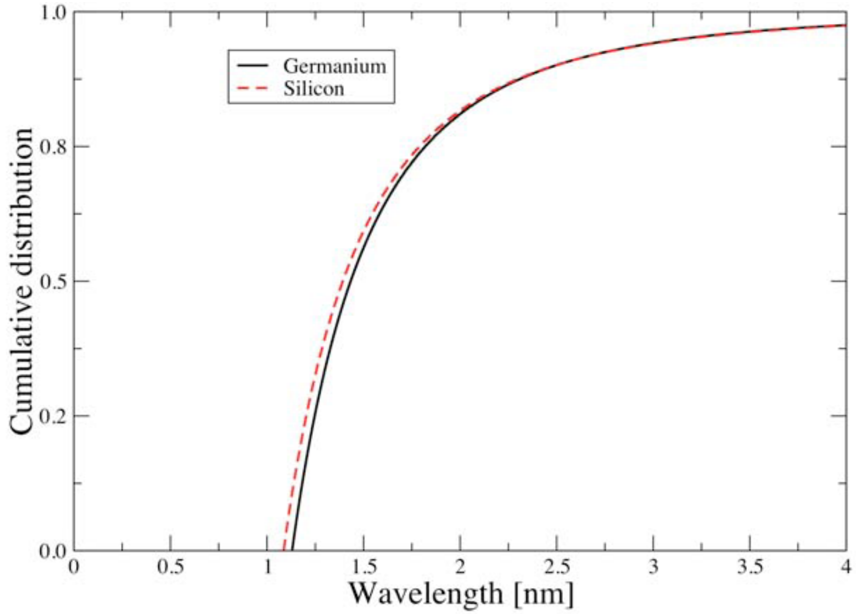




Thermal Conductivity Reduction: Phonon Engineering [1]

Additional phonon scattering at heterointerfaces also modify W-F law improving TE properties



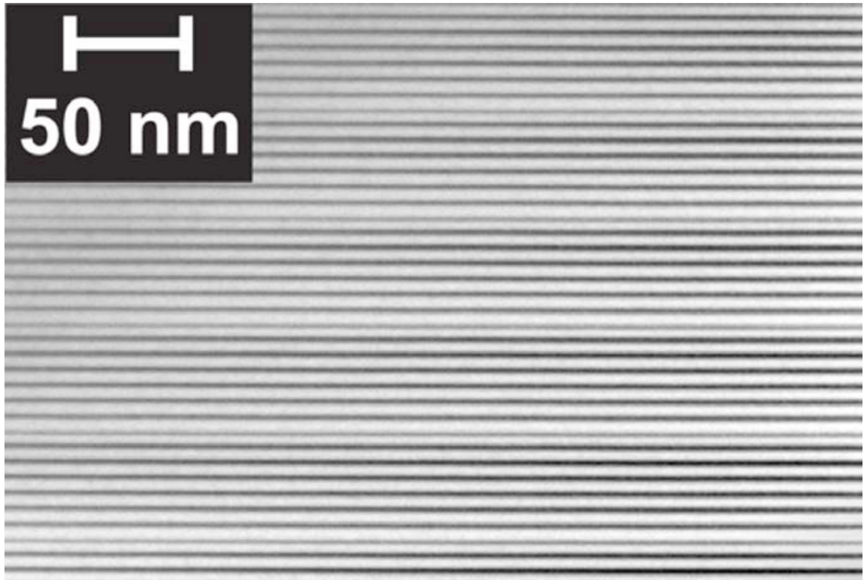


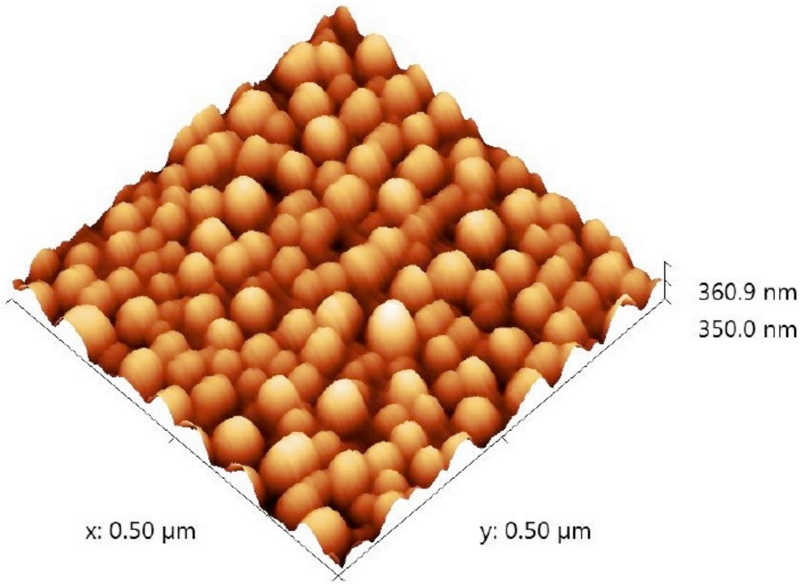
Only 5.92% acoustic phonons have a wavelenght > 3 nm

→ Multiple Ge/SiGe heterolayers to produce **phononic bandgap structures**

[S.T. Huxtable et al. Appl. Phys. Lett. 80, 1737 (2002)]

Thermal Conductivity Reduction: Phonon Engineering [2]





- Use a range of different QWs and barrier thicknesses between 1.2 and 3 nm could block 94.1% of acoustic phonons (short wavelenght acoustic phonons transport more thermal energy due to the higher density of states)

Compared to flat superlattices, nanocrystals (with lateral size of ~10 nm) scatter efficiently also phonons with relatively long wavelengths

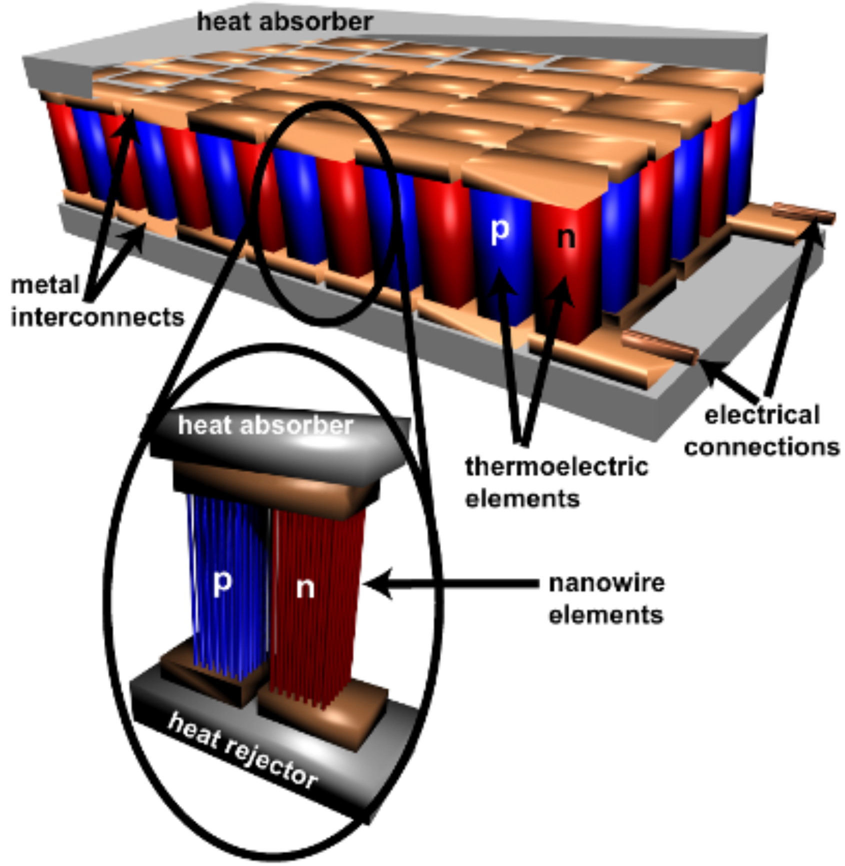
Conclusions

- Low dimensional structures can improve both figure of merit *ZT* and generated power

- With LEPECVD technique it's possible to grow 10 μm Ge/SiGe strain-symmetrised superlattices

- HR-XRD is an indispensable instrument for structures characterization and growth parameters choice

- HRTEM analysis confirmed high quality of material and interfaces grown by LEPECVD



Green Silicon Participants

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ETH Zürich (Switzerland)

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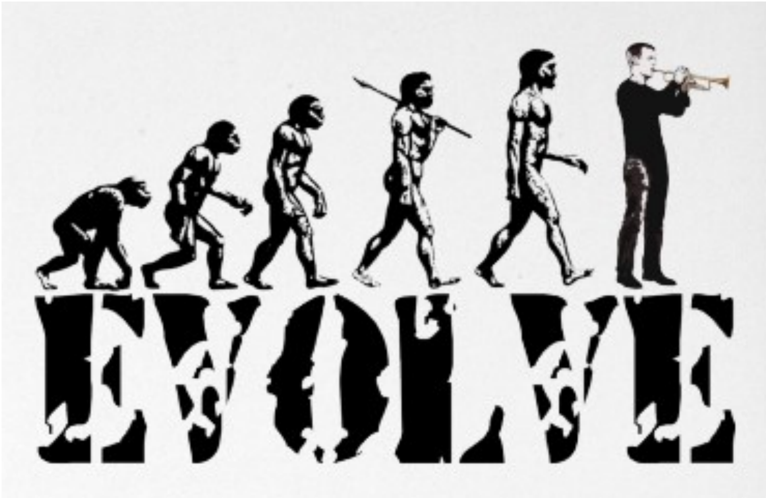
Fabio Isa

Jacopo Frigerio

Daniel Chrastina

Giovanni Isella

Thank you for your attention



...Questions?