Lattice dynamics of epitaxial strain-free interfaces

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Interface-Specific Vibrational Phenomena

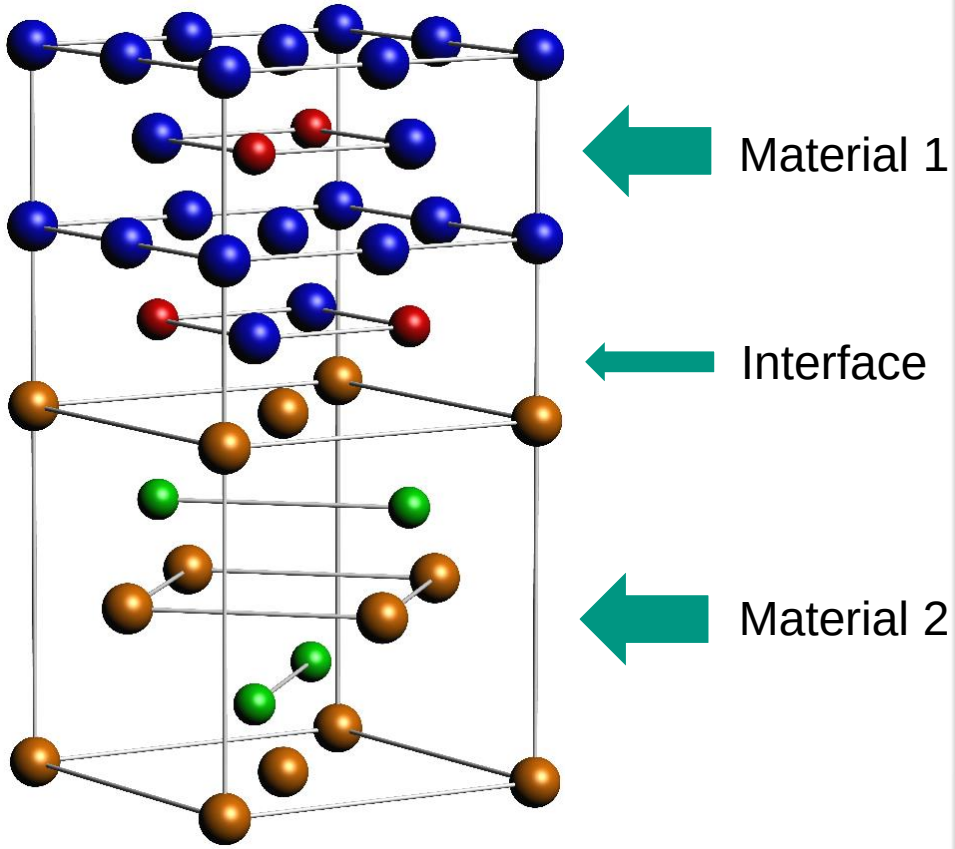
- Phonon folding in superlattices
  C. Colvard et al., Phys. Rev. Lett. 45, 298 (1980)
  C. Colvard et al., Phys. Rev. B 31, 2080 (1985)
  A. K. Sood et al., Phys. Rev. Lett. 54, 2111 (1985)
- Localized vibrational modes

  A. Seiler et al., Phys. Rev. Lett. 117, 276101 (2016)
- Coherent phonon heat conduction

  M. N. Luckyanova et al., Science 338, 936 (2012)
- Crossover from incoherent to coherent phonon scattering

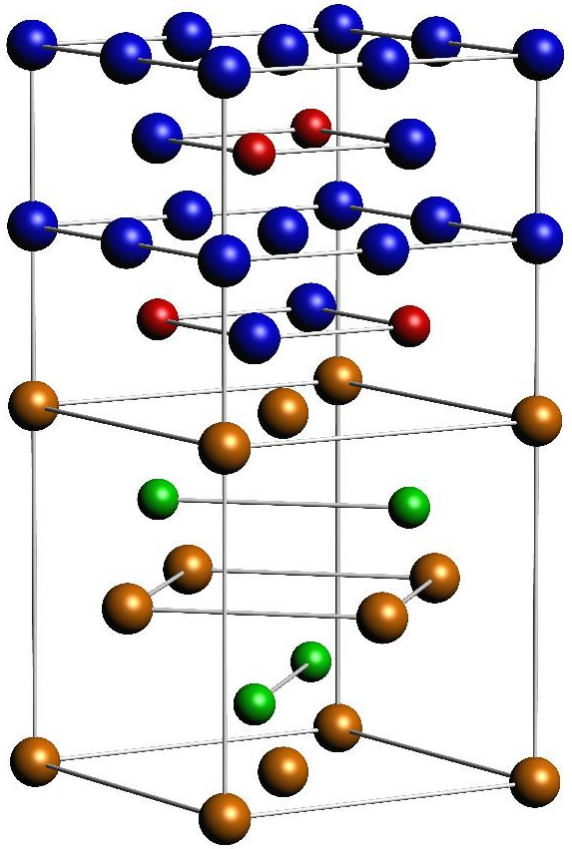
  J. Ravichandran et al., Nat. Mater. 13, 168 (2014)
- Enhanced thermal conductivity

  D. P. Schroeder et al., Phys. Rev. Lett. 115, 256101 (2015)
  W. Park et al., Nanoscale Microscale Thermophys. Eng. 21, 134 (2017)
- ...



Important Questions

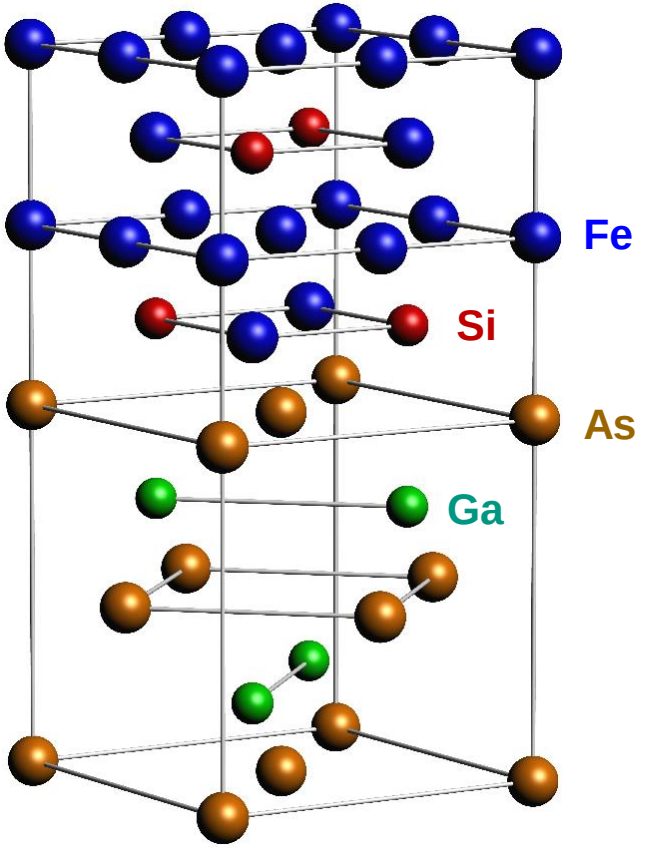
- How are the phonon dispersions / DOS modified at the interface?
- At which distance from the interface bulk lattice dynamics is established?
- Can we achieve a complete qualitative and quantitative picture?



Fe_3Si/GaAs Heterostructures

- Fe_3Si – a simple Heusler alloy
- Spin injection in Si, Ge and GaAs realized
- GaAs provides atomically flat surface
- Fe_3Si/GaAs strain-free interface
- Very well established growth protocol
- Perfect system for Nuclear Inelastic Scattering

  experiments on the Mössbauer isotope ^{57}Fe



A. Kawaharazuka et al., Appl. Phys. Lett. 85, 3492 (2004)
J. Herfort et al., Appl. Phys. Lett. 83, 3912 (2003)
V. Kaganer et al., Phys. Rev. Lett. 102, 016103 (2009)
K. Kasahara et al., J. Appl. Phys. 111, 07C503 (2012)
B. Jenichen et al., Thin Solid Films 556, 120 (2014)
S. Gaucher et al., Appl. Phys. Lett. 110, 102103 (2017)

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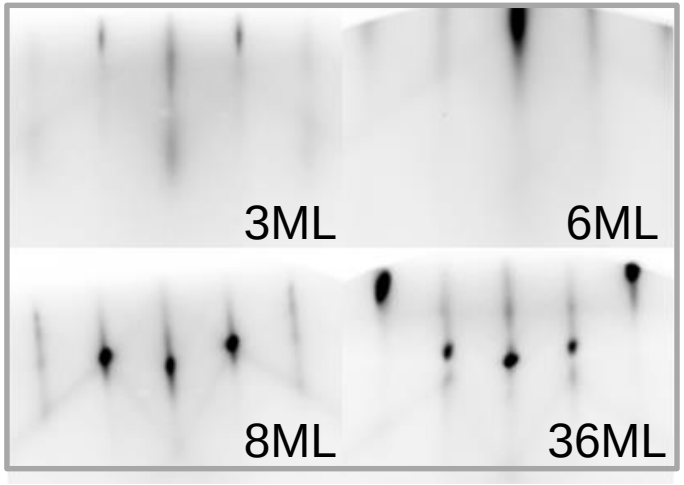
Fe_3Si/GaAs Heterostructures

Molecular Beam Epitaxy

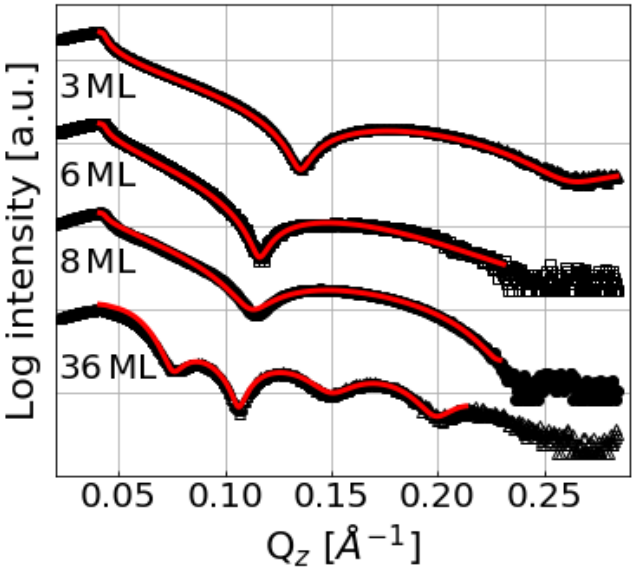
Ge capping layer
Fe_3Si(001) layer
GaAs(001) layer
GaAs(001) substrate

GaAs	Fe_3Si		Ge
350 nm	3 ML	0.85 nm	4 nm
350 nm	6 ML	1.7 nm	4 nm
350 nm	8 ML	2.3 nm	4 nm
350 nm	36 ML	10.2 nm	4 nm

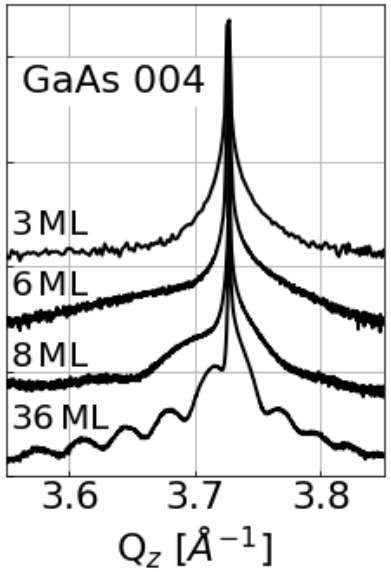
RHEED (Electron Diffraction)



X-Ray Reflectivity



X-Ray Diffraction



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Phonon DOS from Nuclear Inelastic Scattering

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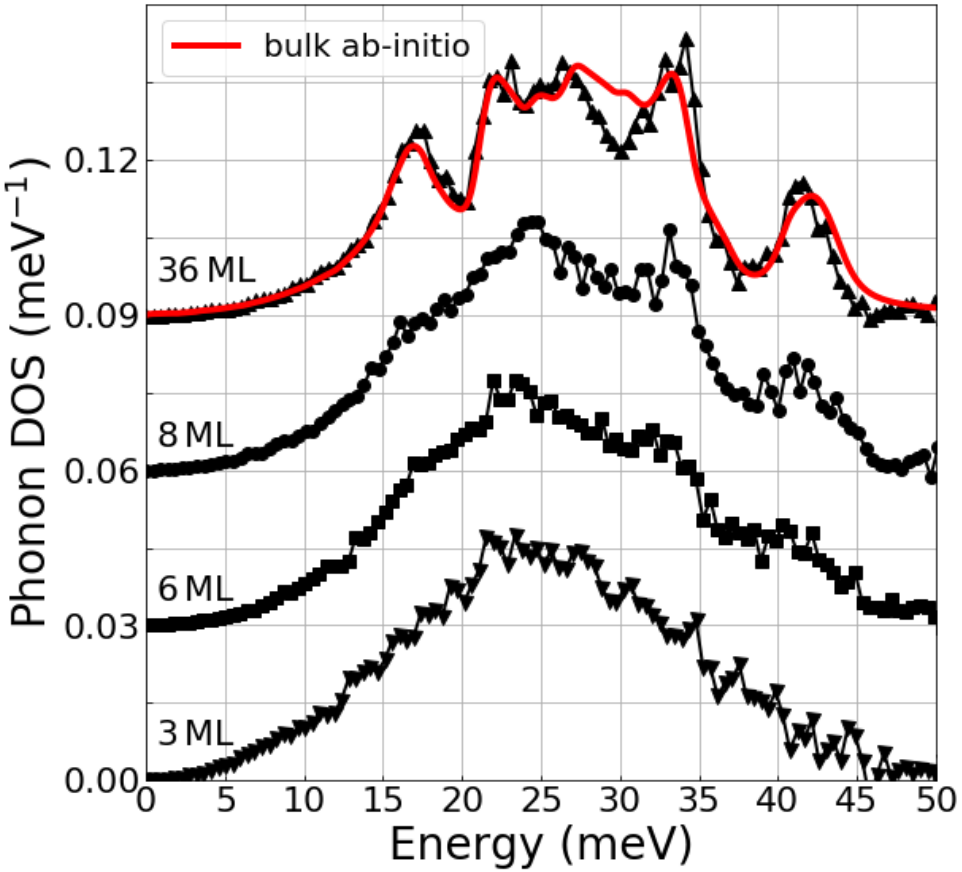
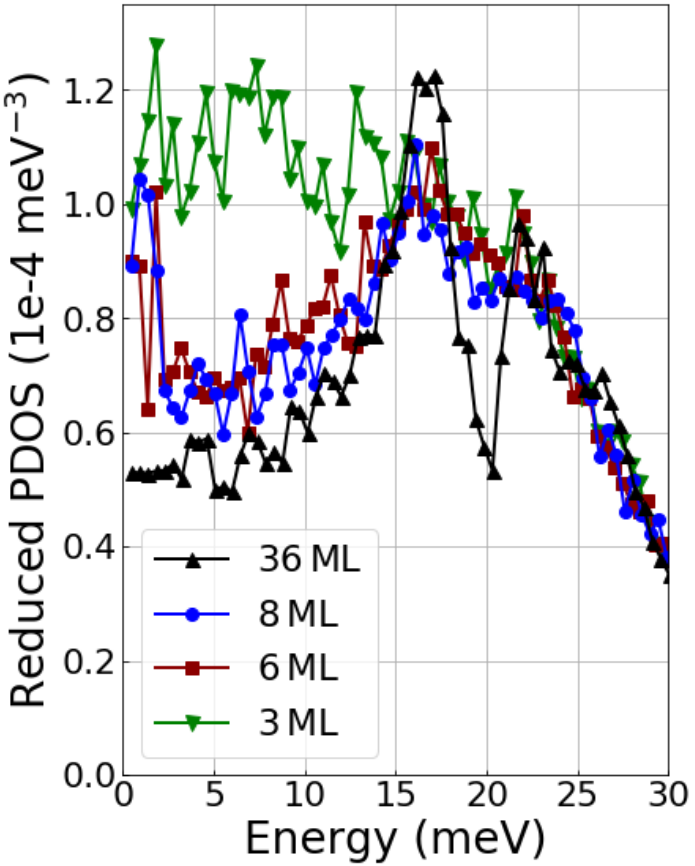
Fe_3Si[100]-projected, Fe-partial PDOS



Reduced PDOS (PDOS/E^2)



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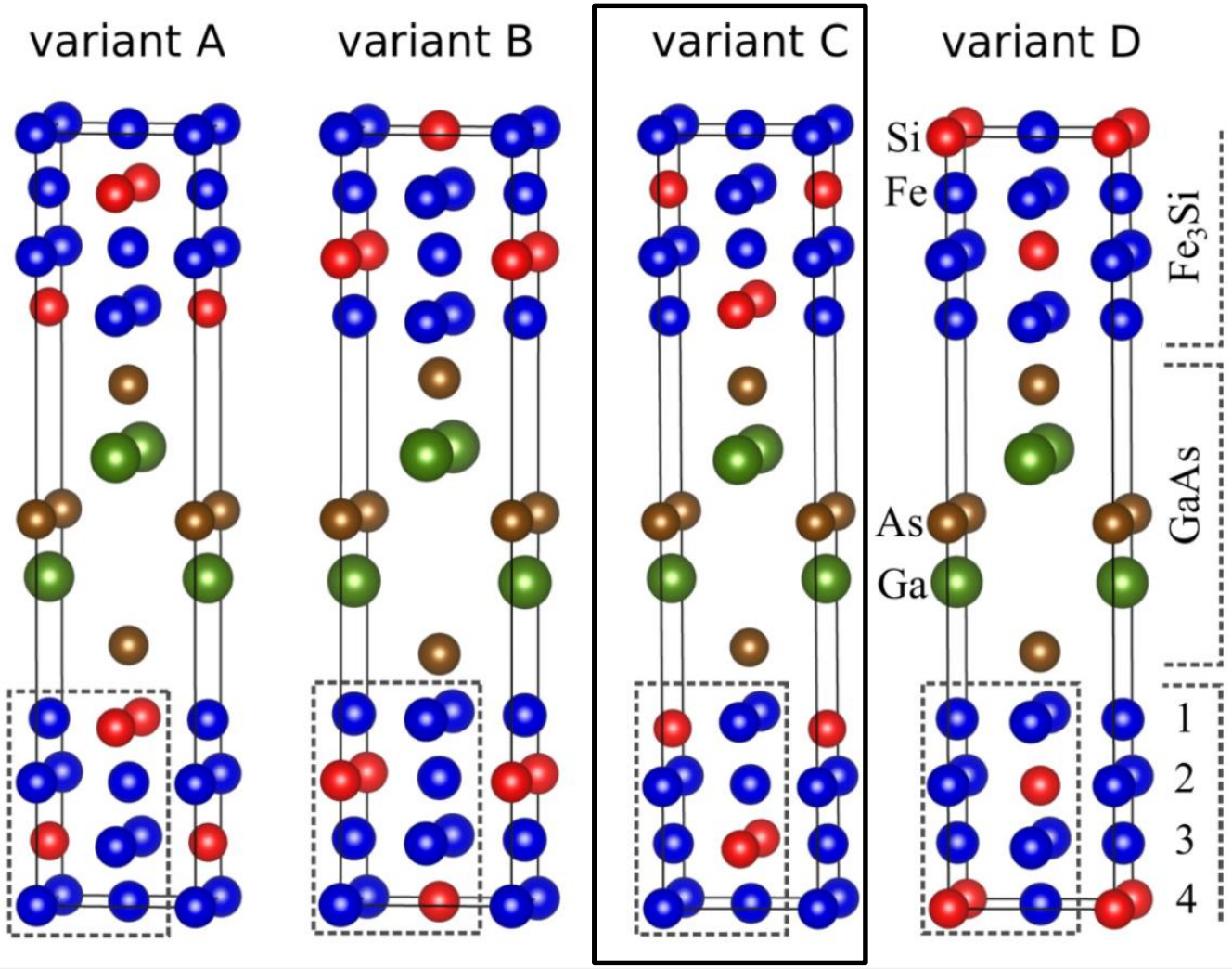
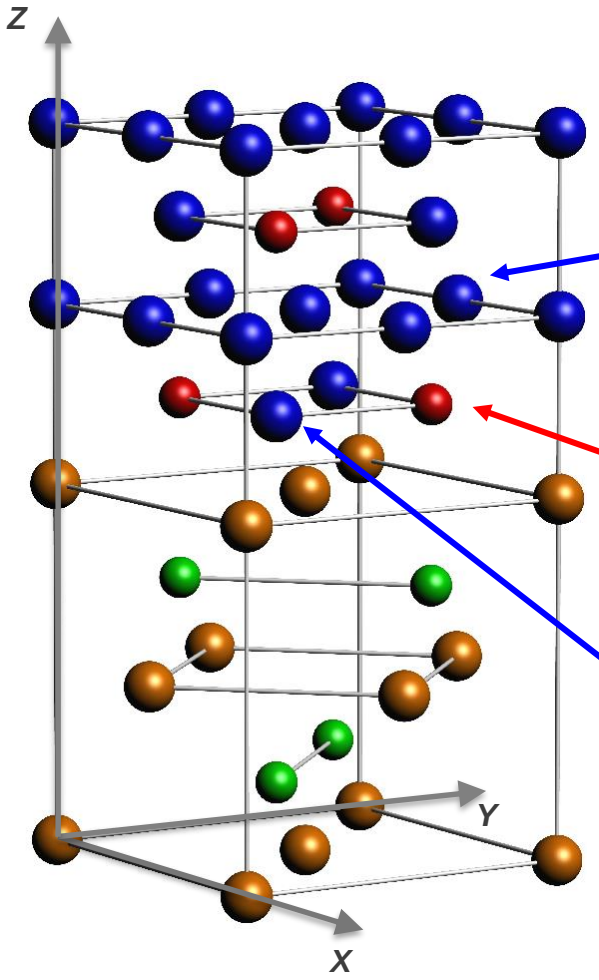
First-Principles Theory

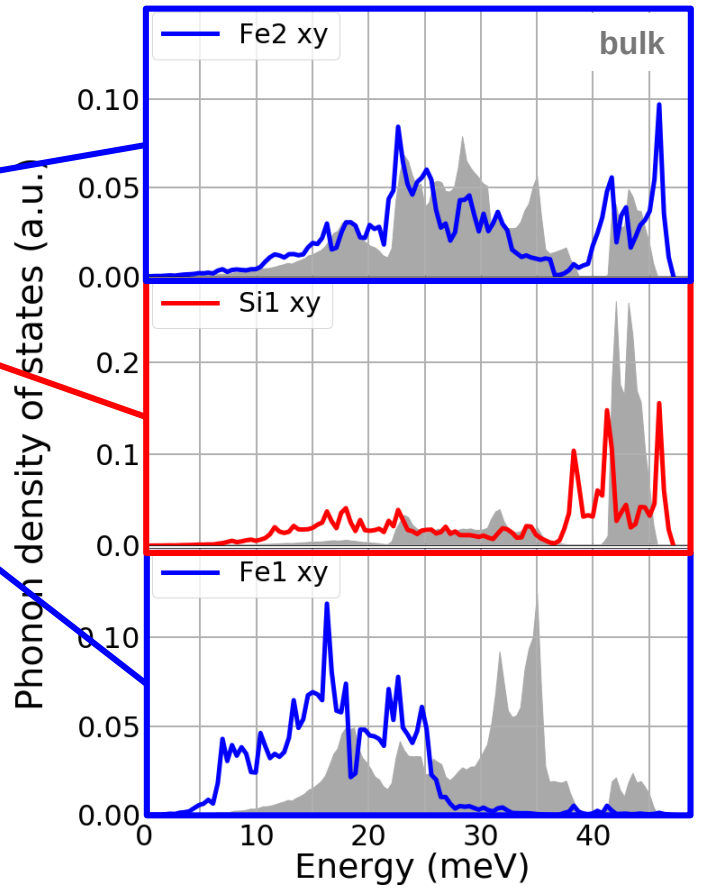


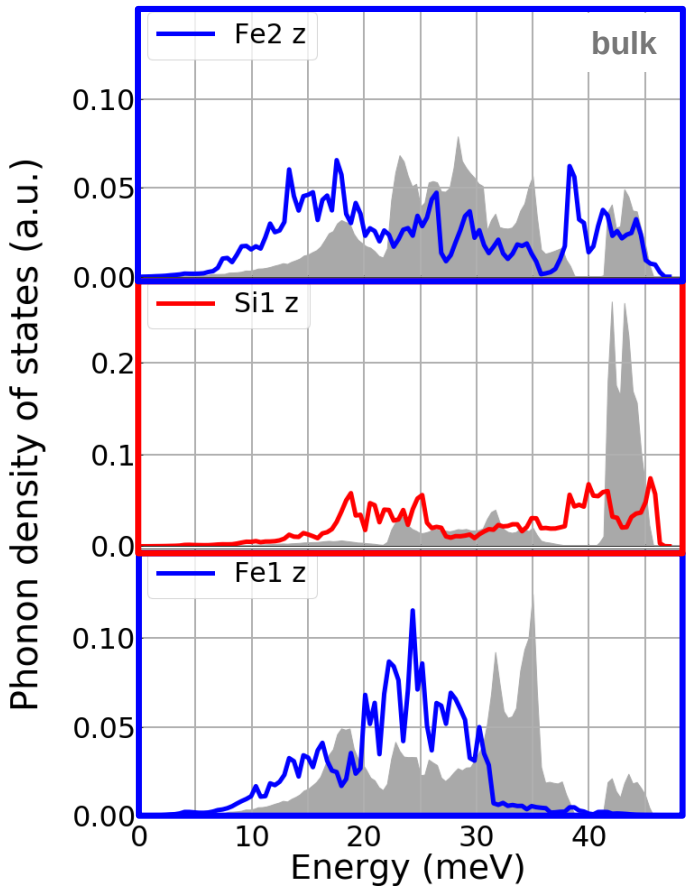
- Following the experimental results only As-terminated GaAs layers were examined
- Due to the periodic boundary conditions a multilayer structure is calculated
- Possible lattice deformations and crystal defects were not taken into account

First-Principles Theory



Element-specific, layer- and polarization-projected PDOS





- Electronic structure is optimized by the VASP code
  G. Kresse and J. Furthmüller, Comput. Mater. Sci. 6, 15 (1996)
- Lattice dynamics is calculated by the direct method implemented in the PHONON code
  K. Parlinski, Z. Q. Li, and Y. Kawazoe, Phys. Rev. Lett. 78, 4063 (1997)

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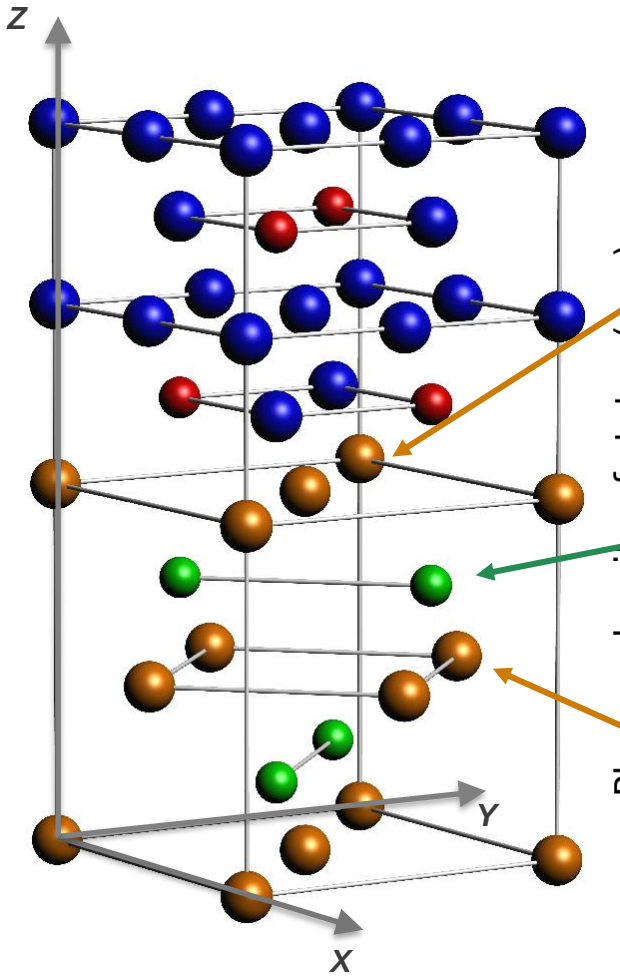
First-Principles Theory



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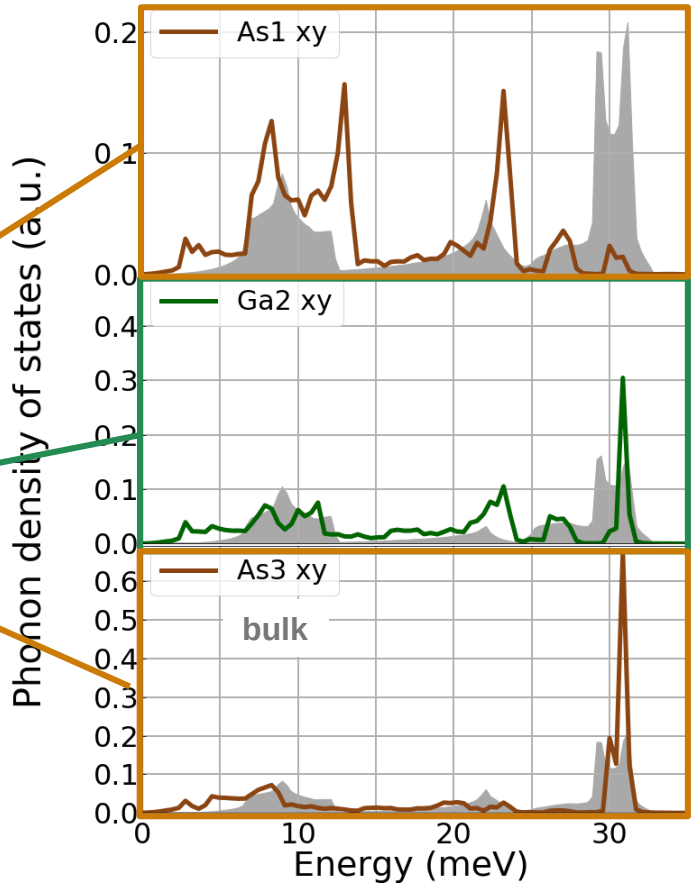

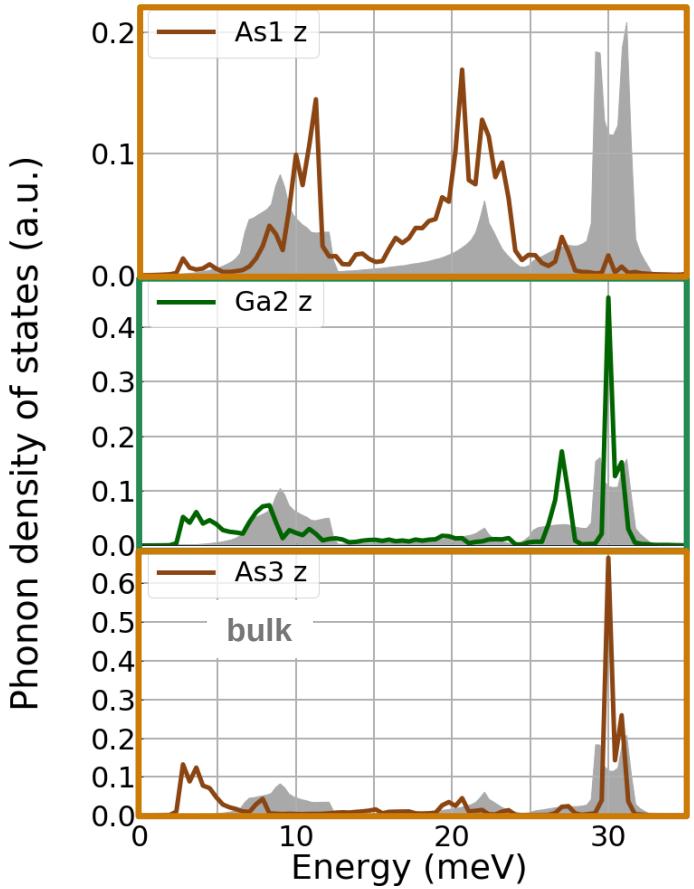

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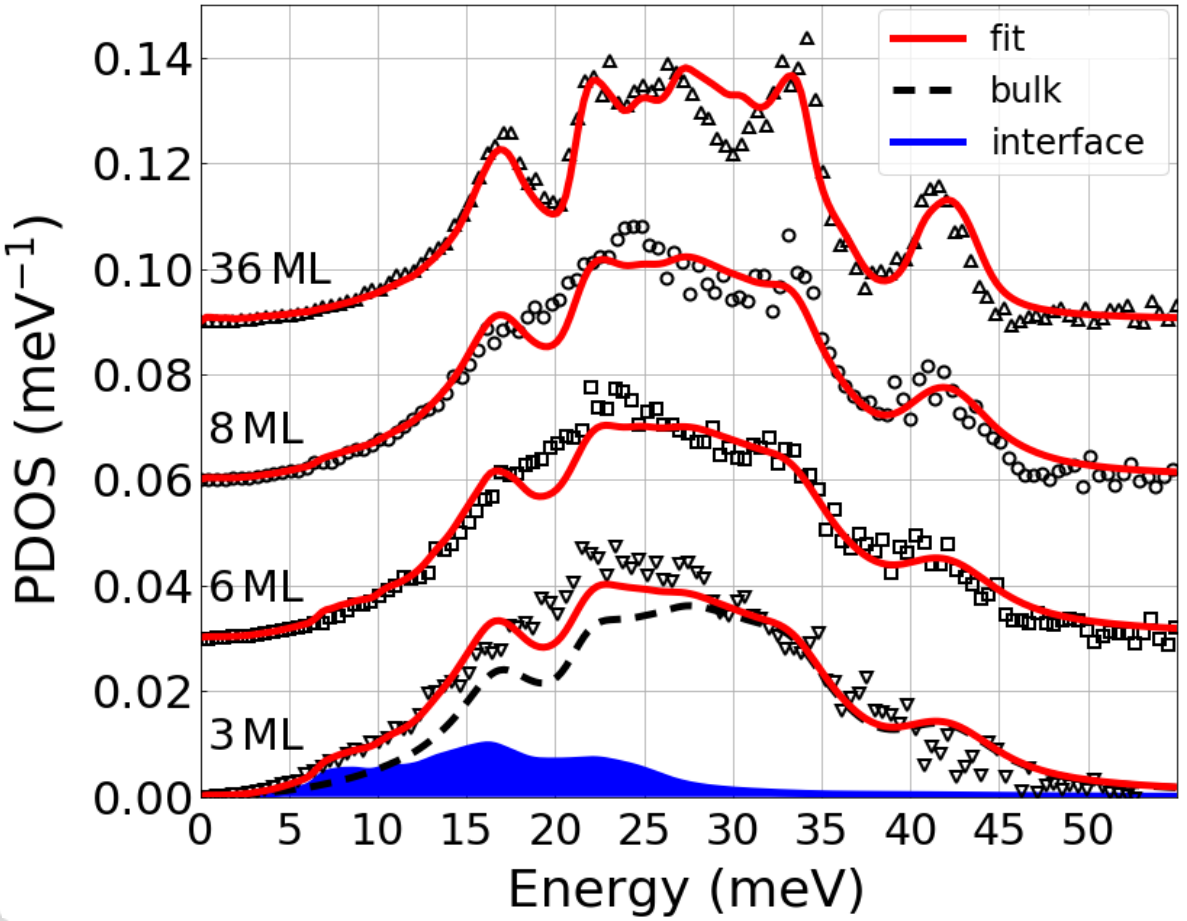
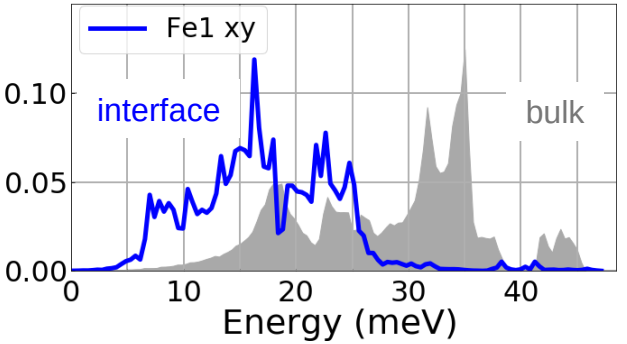
Interface Lattice Dynamics

$$g_{FIT}(E) = A\, g_{IF}(E,Q_{IF}) + (1-A)\, g_{BULK}(E,Q_{BULK})$$

A is the interface atomic fraction
Q is the quality factor of the DHO function





Sample	Q_B	Q_{IF}	A_{FIT} (A_{TEM})
36 ML	21	-	-
8 ML	10	15	0.06 (0.06)
6 ML	7	15	0.09 (0.08)
3 ML	7	8	0.15 (0.14)

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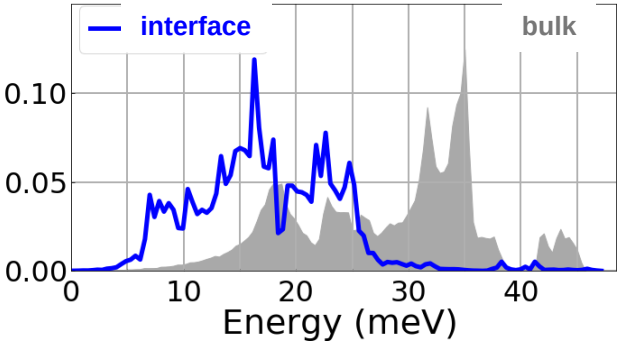
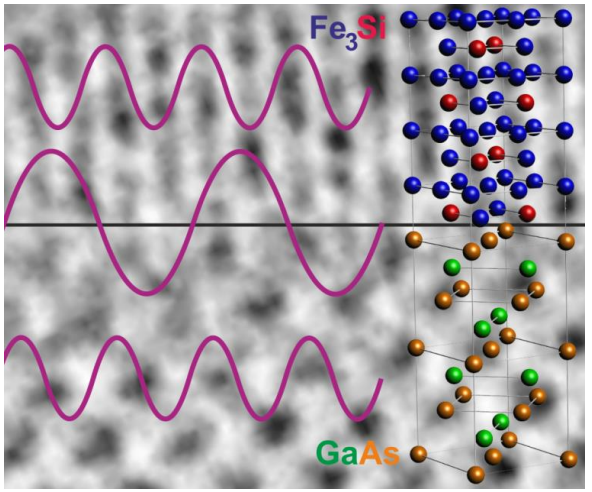
Conclusions & Outlook

- **The lattice dynamics of epitaxial strain-free Fe_3Si/GaAs heterostructure is determined**
- **An interface-specific lattice dynamics is identified (reduced force constants → lower frequencies and higher amplitudes)**
- **The impact of epitaxial strain and materials combination to be explored**
- **Efficient interface phonon engineering in epitaxial multilayers is visible**





***Ab initio* and nuclear inelastic scattering studies of Fe_3Si/GaAs heterostructures**
O. Sikora, J. Kalt, M. Sternik, A. Ptok, P. T. Jochym, J. Łażewski, P. Piekarz, K. Parlinski, I. Sergueev, H.-C. Wille, J. Herfort, B. Jenichen, T. Baumbach, and S. Stankov
Phys. Rev. B 99, 134303 (2019), see also Suppl. Material

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Phys. Rev. B Rapid Comm. 98, 121409 (2018), see also Suppl. Material

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M. Sternik, O. Sikora, P. Piekarz, Institute of Nuclear Physics, Krakow, Poland
- first-principles calculations

I. Sergueev, H.-C. Wille, Dynamics beamline P01, PETRA III, Hamburg
- nuclear resonant scattering experiment

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