Halbleiternanostrukturen: Von den physikalischen Eigenschaften zur Anwendung in der Energieumwandlung und Quantentechnologie

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SiGe pyramid
~20 × 10⁹ smaller than Cheops pyramid
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SiGe pyramid
\[\sim 20 \times 10^9\] smaller than Cheops pyramid
Introduction: the interstellar mission

Voyager 1&2, launched 1977

Work needed: ~130,000 person months (only ~3× smaller than for Cheops pyramid)

Still in touch!

Energy from sun at current location: ~100 mW/m²

Energy source?

Distance of Voyager 1: $18 \times 10^9$ km (~123 AU)

http://voyager.jpl.nasa.gov/
Energy source in deep space

$^{238}\text{PuO}_2$, with half-life 88 yrs

Multihundred Watt Radioisotope Thermoelectric Generator using Silicon Germanium (conversion efficiency $\sim 6.6\%$)

http://voyager.jpl.nasa.gov/
Energy source in deep space

$^{238}\text{PuO}_2$, with half-life 88 yrs

- Direct conversion of heat into electricity
- No moving parts
- No maintenance needed
- Appealing source not only for deep space!

http://voyager.jpl.nasa.gov/
Thermoelectric energy conversion via SiGe

Silicon-Germanium “unicouple”

From http://www.thermoelectrics.caltech.edu/
Thermoelectric energy conversion via SiGe

Silicon-Germanium “unicouple”

Temperature gradient $\rightarrow$ Thermovoltage

$$V = \int_{T_c}^{T_h} \left[ \alpha_p(T) - \alpha_n(T) \right] dT$$

Seebeck coefficients for $n$ and $p$ leg (temperature dependent)

From http://www.thermoelectrics.caltech.edu/
Thermoelectric energy conversion

Efficiency of thermoelectric conversion depends on:

- Seebeck coefficient
- Electric conductivity
- Temperature
- Thermal conductivity
- N-type $e^-$
- P-type $h^+$

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

$ZT$ from 0.2 to 3 in steps of 0.2

$T_h = 1000°C$

Thermoelectric energy conversion

Efficiency of thermoelectric conversion depends on:

- Seebeck coefficient
- Electric conductivity
- Temperature
- Thermal conductivity

\[ ZT = \frac{\alpha^2 \sigma}{\kappa} T \]

Open problems:

- Efficiency generally low → Thermoelectrics relegated to “niche” applications
- Parameters are generally interlinked → material optimization difficult

"Nanostructures": new chance for TE?

Effect of quantum-well structures on the thermoelectric figure of merit

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Department of Electrical Engineering and Computer Science and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 3 December 1992)

Basic idea: use nanostructuring to enhance thermoelectric (TE) conversion efficiency by “decoupling” TE parameters. Size effects are available for additional material optimization.

\[
ZT = \frac{\alpha^2 \sigma}{\kappa} T
\]

thermal conductivity
Nano-SiGe

from G. Joshi et al. Nano Lett. 8, 4673 (2008)


Polycrystalline material: phonon scattering at grain boundaries responsible for drop in \( \kappa \)

Simpler system?
Epitaxial SiGe - Film evolution

Ge deposition on Si: Elastic stress due to 4% lattice mismatch drives film evolution – similar growth mode displayed by other semiconductors
Scanning tunneling microscopy images

4 ML Ge

Scale $180 \times 180$ nm$^2$ (1 ML = 1 Monolayer = 0.14 nm)

Ge on Si(001) @ nominal substrate temperature: 450°C

Layer structure for TE properties studies

- Ge, barrier
- Si, spacer
- Ge, barrier
- Si buffer
- Si (001) Substrate

Molecular beam epitaxy (MBE) growth at substrate temperature of 500°C
Systematic variation of growth parameters, carefully chosen to avoid defects

→ Model system for studying effect of nanostructuring on TE properties
Thin-film thermal resistance measured by 3ω method (Peixuan Chen, JKU) and TDTR (J.P. Feser, D.G. Cahill) - compatible results

\[ \kappa = \frac{\text{film thickness} (N \cdot L)}{\text{thermal resistance}} \]

For the same \( N \), \( R \) increases with Ge amount

Can we eliminate dependence on period number \( N \)?
‘Single barrier’ thermal resistance

\[ R_{\text{tot}} = N R_{\text{barrier}} \]

Ge period \( N \):
- 21
- 81
- 301 (3\( \omega \))
- 301 (TDTR)

Si spacer fixed (6 nm)

Ge barrier thickness (ML)

\( R_{\text{barrier}} \) (10\(^{-9} \) m\(^2\) K W\(^{-1}\))

Crystal Defects

phonon

Si

Ge

R_{\text{barrier}}
Thermal conductivity: Comparison with theory

Average Ge concentration (%)

Exp.: Si 6 nm,
Period number:
- 21
- 81
- 301 (3ω)
- 21
- 81
- 301 (TDTR)

Structures implemented for ab-initio calculations (N. Ayape-Katcho, N. Mingo, CEA Grenoble)
Thermal conductivity: Comparison with theory

Good agreement using realistic composition

→ Real superlattices outperform alloy and also ideal superlattices (with abrupt interfaces)!

Thermal conductivity of dot multilayers

Thermal conductivity values down to 1 W m$^{-1}$ K ($\text{\textquotedblleft} \text{glass\textquotedblright}$ out of single crystalline Ge/Si)

$\kappa = \frac{\text{period length (L)}}{\text{single barrier thermal resistance}}$

G. Pernot et al., Nature Mater. 9, 491 (2010)
Example: InGaAs quantum dots (QDs) on GaAs(001) substrates

**Key features of epitaxial self-assembled QDs:**
- Confine charge carriers in 3D → „artificial atoms“
- Compatible with optoelectronic devices → hardware for quantum communication?

Envisioned applications of single QDs

Secure data communication via quantum cryptography

Classical channel (e.g. optical fiber)

Quantum channel for key distribution (optical fiber or free space)

Sender: Alice  
Receiver: Bob

Eavesdropper: Eve 😊

Eavesdropper: Eve 😞

Bits (qubits) of secret key encoded in the polarization state of a photon

Any attempt of Eve to measure the key will perturb the result (wavefunction collapse), which can be detected by Bob and Alice

For long distance communication amplifiers (A) for classical channel and quantum repeaters (QR) for quantum channels necessary to compensate losses

New hardware required! Can this be QD-based?

See Mark Fox, Quantum Optics – An Introduction, Oxford Univ. Press (2006)
Epitaxial QDs and their basic properties

Example: InGaAs QDs on GaAs(001) substrates

Atomic force microscopy topograph of QDs on surface

scale 1400x700x12 nm³

Emission spectrum of an ensemble of InGaAs QDs

Ground state

1st excited state

~10-30 meV

Wavelength (µm)

Key features of epitaxial self-assembled QDs:

• Confining charge carriers in 3D → artificial atoms
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• Shape/size/composition fluctuations → each QD has its own energy spectrum

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Emission spectrum of 2 nearby QDs

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• Need for post-growth tuning methods!
Epitaxial QDs and their basic properties

Example: InGaAs QDs on GaAs(001) substrates

Atomic force microscopy topograph of QDs on surface

Transmission electron micrograph of a QD embedded in GaAs matrix

Key features of epitaxial self-assembled QDs:
• Confine charge carriers in 3D $\rightarrow$ artificial atoms
• Compatible with optoelectronic devices $\rightarrow$ hardware for quantum communication?
• Shape/size/composition fluctuations $\rightarrow$ each QD has its own energy spectrum
• Need for post-growth tuning methods!
QDs as sources of indistinguishable photons

Optically pumped QD under variable vertical electric field →
quantum confined Stark effect allows energy tuning

QD in resonant cavity LED (RC-LED) ~not tunable

see also: E.B. Flagg et al. Phys. Rev. Lett. 104, 137401 (2010) - strain provided by PZT used for energy tuning in narrow range (~40µeV)
Hybrid semiconductor-piezoelectric devices

A resonant-cavity diode membrane integrated on piezo

Single-crystal PMN-PT $\left[ \text{Pb(Mg}_{\frac{1}{3}}\text{Nb}_{\frac{2}{3}}\text{O}_3 \right]_{0.72-\left[ \text{PbTiO}_3 \right]_{0.28}}$ capable of $\varepsilon_{//}$ up to $\sim \pm 0.2\%$ at low temperature


First work with QDs and PMN-PT: T. Zander et al., Optics Express 17, 22452 (2009)
Device cross-section and top view

SEM after focused ion beam cut

Optical microscopy view of 100x120 µm² membrane diode

- TiO₂
- SiO₂
- Active layer
- QDs
- PMN-PT
- 200 nm

- Au bonding layer / mirror / electrical contact
- Planar cavity enhances extraction efficiency by about 20x

Strain-tunable QD-LED (frequency stabilized)

Electroluminescence spectra of a single QD upon compression

Part of the emitted light is used for providing a feedback to the piezo → Computer-controlled, wavelength-tunable, quantum emitter in LED
Strain-tunable QD-LED

V_d used to control current in diode (→EL intensity)

V_p controls emission energy shift (>20 meV)

XX-X crossing


F. Ding et al., PRL 104, 067405 (2010)
Energy stability

\[ E_r = 1.3955 \text{ eV} \]

\[ \mu \text{eV stabilization easily reachable with spectrometers} \]

\[ \frac{\text{Range}}{\text{Precision}} \sim 20.000 \]

Triggered single-photon emission?

Single-photon detectors [Image of a 50:50 beam splitter]

\[ \Delta t \text{ histogram} \]

\[ \rightarrow \text{Single photon emission shows up as a lack of coincidence events at } \Delta t = 0 \]

For first demonstration see Science 295, 102 (2002)
Triggered single-photon emission

\( g^{(2)}(0) = 0.11 \)
\( g^{(2)}(0) = 0.10 \)
\( g^{(2)}(0) = 0.08 \)
\( g^{(2)}(0) = 0.07 \)

200 MHz modulation frequency (300 ps pulses)

J. Zhang, F. Ding, E. Zallo, R. Trotta, B. Höfer, L. Hang, S. Kumar, A. Rastelli, O. G. Schmidt (2013)
Diodes in reverse bias

PMN-PT

Exciton (X)
Electro-elastic tuning in “additive mode”

Energy tuning range extended to >30 meV by adding electric and strain fields

1) Drive X to predefined energy and lock via piezo
2) Ramp electric field to decrease XX binding energy and actively *compensate* X shift via piezo.

**Conclusions & perspectives**

**Ge/Si multilayers as model nanostructured thermoelectrics system**

- Single-crystalline material with tunable thermal conductivity (down to 1 W/m·K)
- Crucial role of Ge surface segregation

- Other thermoelectric parameters?
- Other materials?

**Strain-tunable QD devices**

- New tunable optoelectronic devices: triggered single-photon and entangled photon sources...

- Add more knobs?
- New quantum optics experiments with tunable QDs?
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