New CMOS-Compatible Materials for Efficient Infrared Light-Absorption and Emission

Dr. Carlos Augusto

IEEE Nanotechnology Council

March 14, 2024

Problem

The one optical component that has not yet been built into a silicon IC is a compelling, high-performance silicon-based laser. There have been several attempts at making a laser out of silicon, but no technology has yet proved to be commercially viable. The only solution is to use InP EELs.

- "Market and technologies trends for PICs", Eric Mounier, PhD, YOLE INTELLIGENCE

https://medias.yolegroup.com/uploads/2023/04/slides-yole-pic-2023-public_eric-m.pdf

Solution

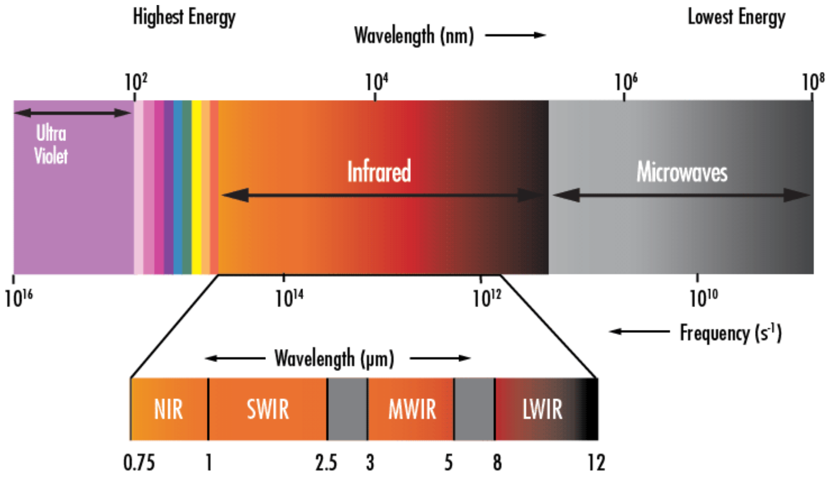
Quantum Semiconductor's disruptive material technology

Paradigm-Shift for IR Absorption & Emission in CMOS

Monolithic Integration, More Functionality, Lower-Cost, Higher Reliability

Quantum Semi has patented engineered Group-IV Superlattices (SLs)

- Direct bandgaps in the Infra-Red (SWIR, MWIR, LWIR).
- Suitable for both imaging and photonics - light absorption and emission in one chip.
- High sensitivity in the SWIR range (from 0.8µm to 2.5µm).
- Projected Better Quantum Efficiency at 1550nm than InGaAs or Ge.
- Feasible to fabricate with 300mm epitaxial equipment used in CMOS.
- Over 1500 compositions studied with proprietary ab-initio software.
- Nearly perfectly strain-balanced to silicon (no buffer layers).
- Atomistic engineered materials.
- Optoelectronic properties robust to composition variations.
- Group-IV elements compatible with CMOS.
- Leverages existing Si microelectronics supply chain.



Advantages of SWIR in Imaging and Lasers

Comparison of Wavelength range:

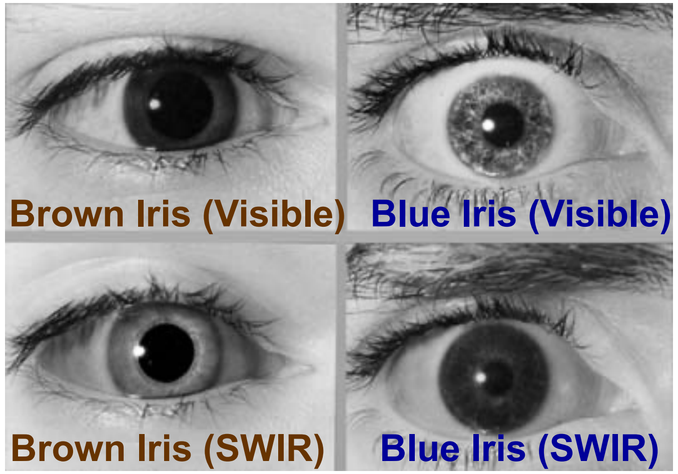
- **QS Superlattice: ~2.7 µm**
- **$In_{0.53}Ga_{0.47}As$: ~1.7µm**
- **Germanium: ~1.8µm**

Only QS Superlattices can use the entire Night-Glow resulting in **Better Night Vision** than InGaAs or Ge.

Enhanced Safety with SWIR

Source: https://www.sensorsinc.com/applications/military/night-vision-systems/

Biometrics & Medical Monitoring



Smaller Pixels and **Higher Quantum Efficiency of sensing at 1.55µm** than InGaAs or Germanium.

Extended eye-safe IR-LiDAR @1550nm allows **500X more Laser Power** than @940. See farther.

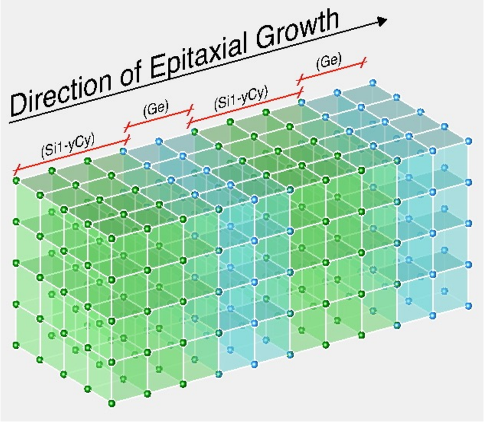
Our Differentiators

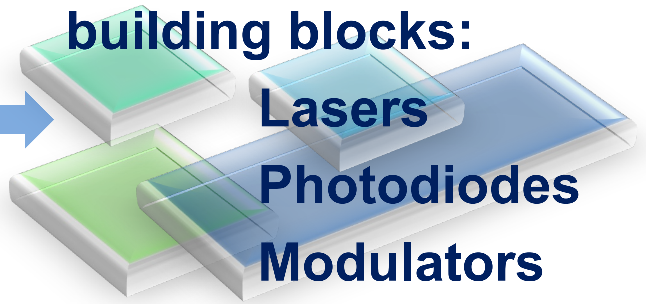
Single-chip with 2D array of Pixels + Lasers: unmatchable small Size, low Weight and Power

Quantum Semiconductor's **Monolithic Integration** technology overcomes the challenges of Heterogeneous Integration of III-V Lasers into Silicon Photonics.

- Same fabrication cost for 1 or 1 million LASERs:
  - High redundancy can be used to increase yield and lifetime of products.
- 2D Arrays of LASERs coherently combined for:
  - More optical power (e.g., useful for LiDAR).
  - Better heat dissipation of spatially distributed LASERs.
  - Beam steering and all optical switching.
  - Enables massively parallel photonic AI.

- All photonic devices built with Group-IV materials.
- High integration density next to CMOS devices.
- Lower parasitics.
- Tracks Moore's Law.
- No assembly or alignment needed.
- Low-cost manufacturing via epitaxy on 300mm wafers.
- Takes advantage of CMOS processing (lithography, deposition, etching, etc.) for high yields & lower cost.





Photonic circuit building blocks:

Lasers

Photodiodes

Modulators

Transceivers

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Quantum Semiconductor’s Disruptive Technology

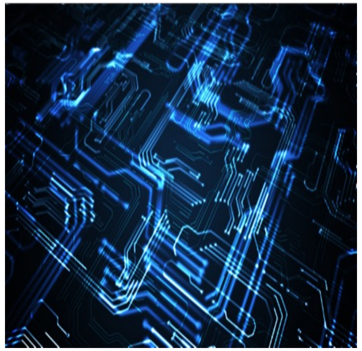
Special materials – Patented compositions – High barrier to entry – Unique specialization needed

Fundamental technology innovations revolutionizing 4 Key Markets:

- **Silicon Photonics**: Monolithic Integration of Lasers and Photodiodes into CMOS.
- **AI and HPC:** Datacom photonic links to CMOS, arrays of lasers for neuromorphic computing.
- **LiDAR**: Monolithic Integration of Lasers and Photodiodes into CMOS for beam-steering in one chip.
- **SWIR Imaging**: Low-cost & high-performance leveraging existing silicon supply chain for BSI and FSI.

Silicon Photonics

TAM of $1B (2027)

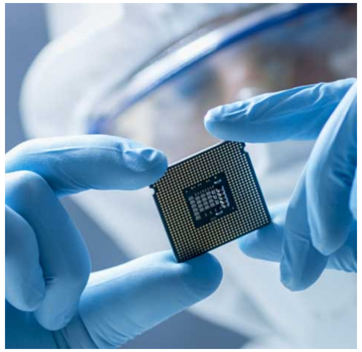


AI and Data Center HPC

TAM of $2.6B (2033)

Single Chip LiDAR

TAM of $4.8B (2028)



Sensors and Detectors

TAM of $29B (2028)

https://www.yolegroup.com/product/report/silicon-photonics-2023/

https://www.yolegroup.com/product/report/co-packaged-optics-for-datacenter-2023/

https://www.yolegroup.com/product/report/lidar-for-automotive-2023/

https://www.yolegroup.com/product/report/swir-imaging-2023/

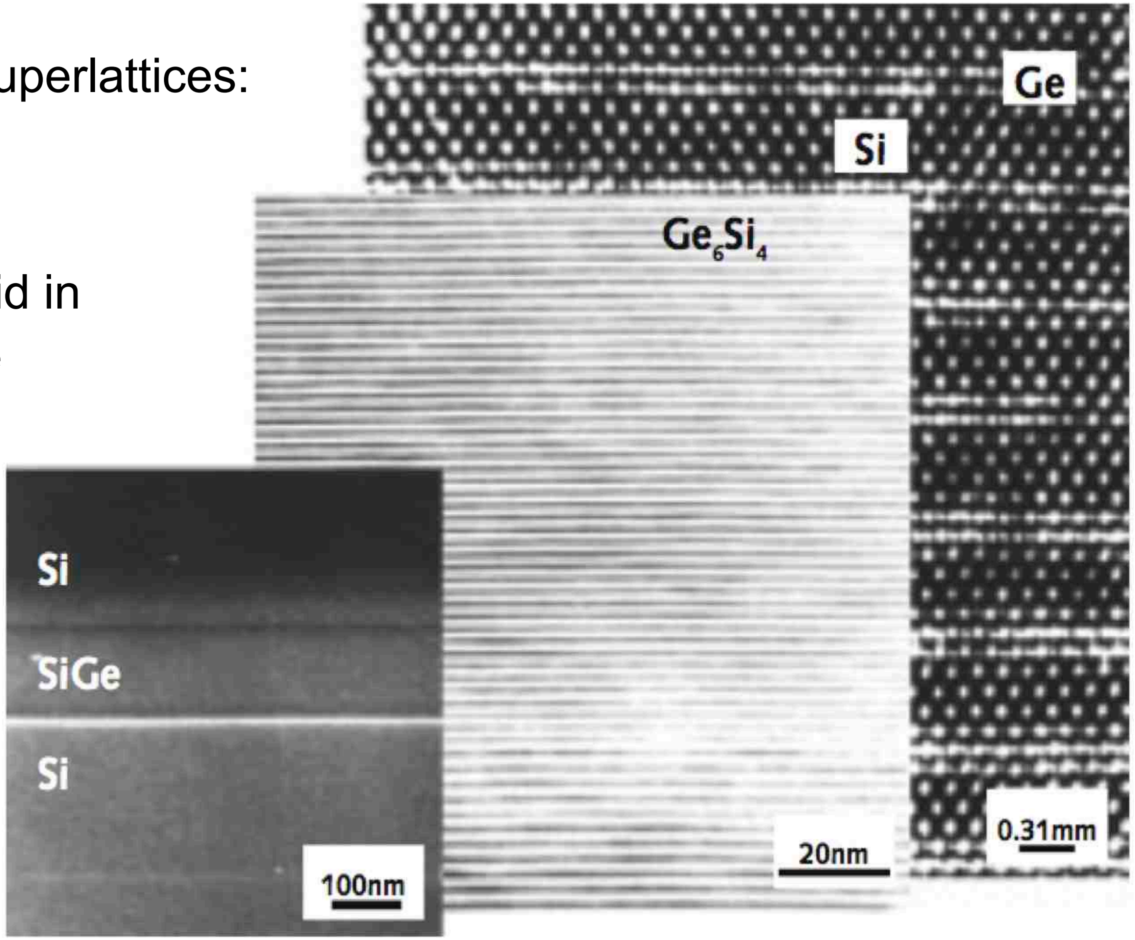
History of Group IV Superlattices: 1980s and 1990s

1974: Brillouin Zone Folding in Si-Ge superlattices to engineer direct band-gaps:
U. Gnutzmann & K. Clausecker: “Theory of direct optical transitions in an optical indirect semiconductor with a superlattice structure”; DOI: 10.1007/BF00892328.

1980s: Experimental and theoretical work on Short-Period Superlattices:
Si-Ge only, no Carbon.

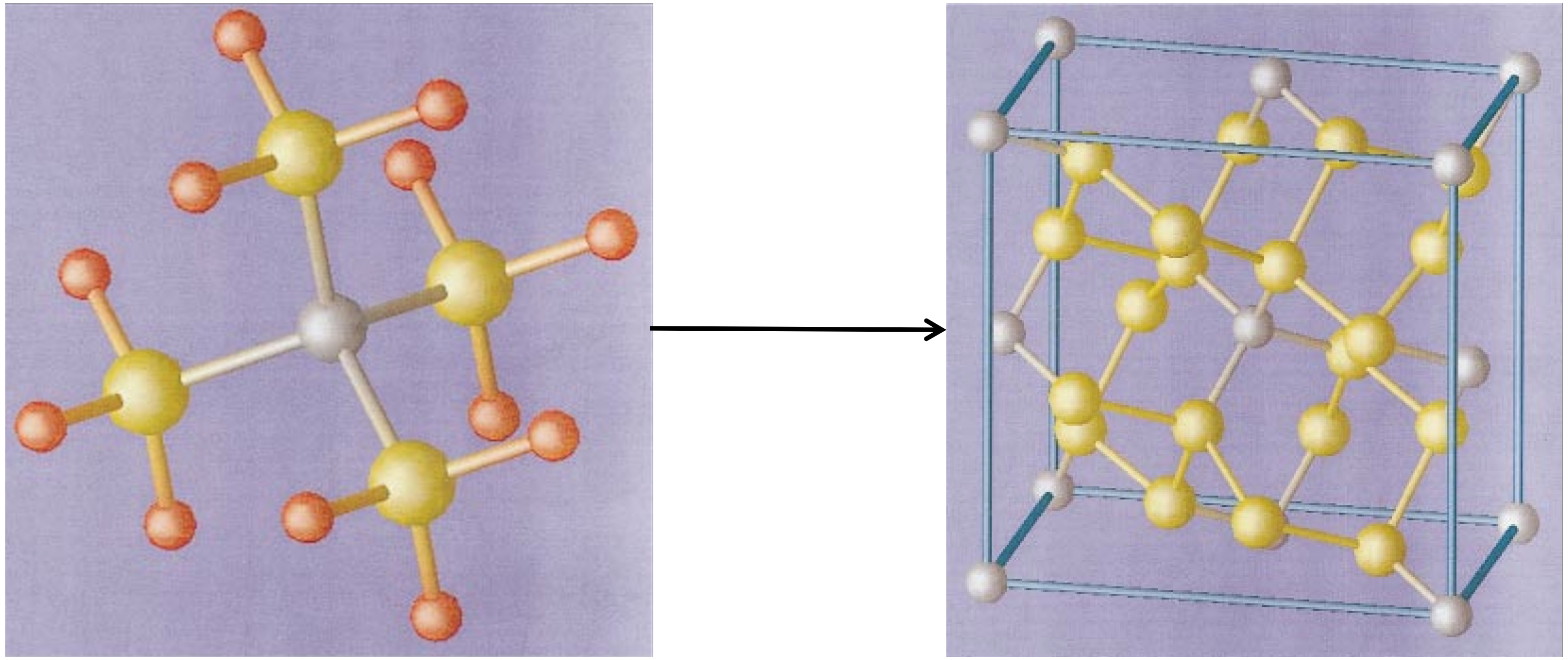
1990s: Addition of Carbon to SiGe in small percentages to aid in strain compensation. Carbon content (< 4%) not able to be increased due to equipment limitations.

Group of H.-J. Osten at IHP produced one-of-a-kind results with Carbon that were never replicated: S. Ruvimov, E. Bugiel, H.-J. Osten, “Structural characterization of Si_nC δ layers embedded in a silicon matrix”.
J. Appl. Phys. 1995; 78:2323. DOI: 10.1063/1.360149



Group-IV Specialty Precursors for Epitaxy by CVD

- Work on advanced group-IV alloys was demonstrated by J. Kouvetakis et al, "**Growth and characterization of thin $Si_{80}C_{20}$ films based upon Si_4C building blocks**", (1998); DOI:101063/1.120876.
- Ab-Initio simulations of materials enabled by these precursors: P. Zhang, et al, **"Theory of metastable group-IV alloys formed from CVD precursors",** (2001); DOI: 10.1103/PhysRevB.64.235201.



Precursor: $C(AX_3)_4$ (A=Si, Ge, or Sn)

Crystal: Si_4C, Ge_4C, or Sn_4C

- By this time, it was already known theoretically why Si_m-Ge_n SLs strained to Si or Ge, could not have direct band-gaps.
- Only Si_m-Ge_n strained to SiGe relaxed buffer layers could have direct band-gaps.
- Thick buffer layers (typically > 1µm) made it difficult for CMOS integration of these SLs.

Group-IV Atomic Layer Epitaxy

- Self-limiting growth or “Digital Epitaxy” demonstrated for Si, Ge, B- & P-doping in Si and Ge.
- Using CVD, in some cases with commercial equipment for 200mm wafers (ASM Epsilon).
- Work mostly from the group of J. Murota et al, (2011) DOI: [10.1166/jnn.2011.5052](https://doi.org/10.1166/jnn.2011.5052).

MUROTA LAB. RIEC, Tohoku Univ.

innovations for high performance microelectronics

Atomically Controlled Processing for Silicon-Based CVD Epitaxial Growth

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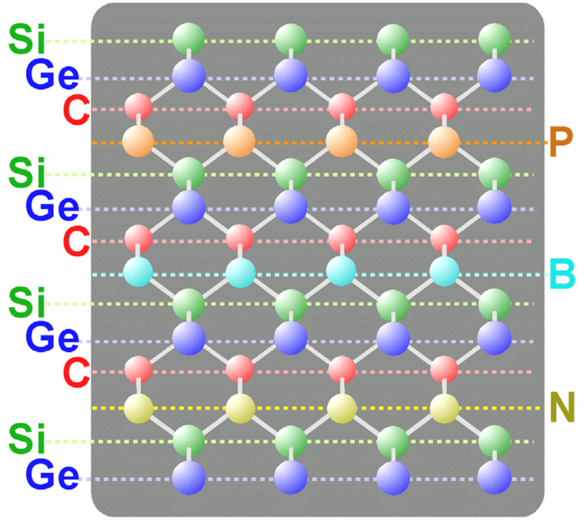
[2] IHP, Germany

[3] Technische Universität Berlin, Germany

Atomic-Layer Superlattice Structure of Si, Ge, C, P, B and N (Target)



- Band Engineering for Group IV Semiconductor
- High Mobility and High Carrier Concentration

2010s: Epitaxy of Layers with High Carbon %

Self-limiting growth of SiC monolayer (delta-layer) in Ge/SiC/Ge stacks

- Demonstration of SiC δ-layers: Si & C atoms in different sub-monolayers (Zinc-Blende crystal).
- Self-limiting growth at low temperature: ~350 C
  Stable up to ~550 C.
- Carbon is incorporated in a deterministic ratio:
  - Precursor with desired % of C (e.g., 50%)
  - Adsorption of the $H_3C\text{-}SiH_3$ molecule
  - Suppression of C out-diffusion with N_2 ambient
  - Ordered C incorporation does not degrade mobility
- Ge offers strain-balance to C layers with high %.
- Work done with commercial CVD equipment for 200mm wafers (ASM Epsilon).

Contents lists available at ScienceDirect

Thin Solid Films

journal homepage: www.elsevier.com/locate/tsf

ELSEVIER

C and Si delta doping in Ge by CH_3SiH_3 using reduced pressure chemical vapor deposition

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ARTICLE INFO

Article history:
Received 30 April 2015
Received in revised form 19 September 2015
Accepted 21 September 2015
Available online xxxx

Keywords:
Chemical vapor deposition
Germanium
Methylsilane
Atomic layer doping
Delta layer

ABSTRACT

C and Si delta doping in Ge are investigated using a reduced pressure chemical vapor deposition system to establish atomic-order controlled processes. CH_3SiH_3 is exposed at 250 °C to 500 °C to a Ge on Si (100) substrate using H_2 or N_2 carrier gas followed by a Ge cap layer deposition. At 350 °C, C and Si are uniformly adsorbed on the Ge surface and the incorporated C and Si form steep delta profiles below detection limit of SIMS measurement. By using N_2 as carrier gas, the incorporated C and Si doses in Ge are saturated at one mono-layer below 350 °C. At this temperature range, the incorporated C and Si doses are nearly the same, indicating CH_3SiH_3 is adsorbed on the Ge surface without decomposing the C—Si bond. On the other hand, by using H_2 as carrier gas, lower incorporated C is observed in comparison to Si. CH_3SiH_3 injected with H_2 carrier gas is adsorbed on Ge without decomposing the C—Si bond and the adsorbed C is reduced by dissociation of the C—Si bond during temperature ramp up to 550 °C. The adsorbed C is maintained on the Ge surface in N_2 at 550 °C.

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Please cite this article as: Y. Yamamoto, et al., C and Si delta doping in Ge by CH_3SiH_3 using reduced pressure chemical vapor deposition, Thin Solid Films (2015), http://dx.doi.org/10.1016/j.tsf.2015.09.046

Group-IV Superlattices: Epitaxial Growth

- **Key Factors for repeatable and reliable epitaxial growth:**
  - Advanced 300mm epitaxial CVD reactors used in leading edge CMOS (FinFETs and GAA Nanosheet FETs).
  - This equipment is available at leading edge foundries (Intel, TSMC, Samsung, GlobalFoundries).
  - ASM Intrepid ES or AMAT Centura Prime Epi cluster tools.
  - Production precursors for Si, Ge and C, are qualified for high volume production.

INTREPID® ES™

- isothermal reactor with closed-loop quartz temperature control
- dual pyrometer/ TC temperature measurement
- low chamber volume
- high throughput

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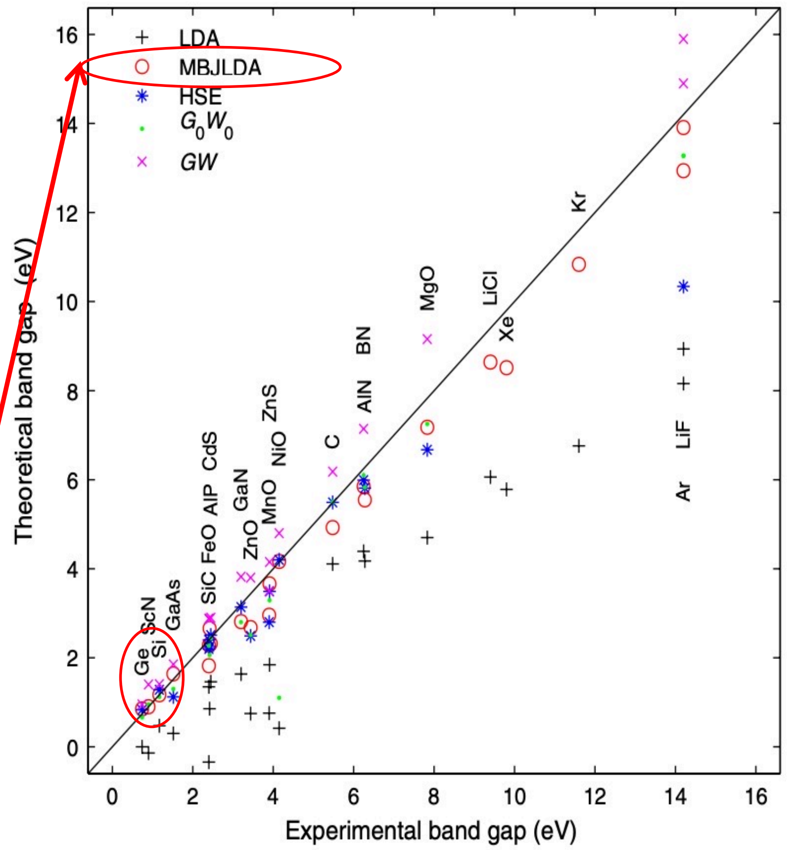
Ab-Initio Simulations and Accuracy

- **DFT simulations agree with experimental data of nano-engineered Group-IV materials**

  E.M.T. Fadaly, A. Dijkstra, J.R. Suckert, et al:
  “**Direct-bandgap emission from hexagonal Ge and SiGe alloys**”,
  Nature **580,** 205–209 (2020); DOI:10.1038/s41586-020-2150-y.
  Editorial in Nature: DOI: 10.1038/d41586-020-00976-8,
  “**Nanostructured alloys light the way to silicon-based photonics**”.

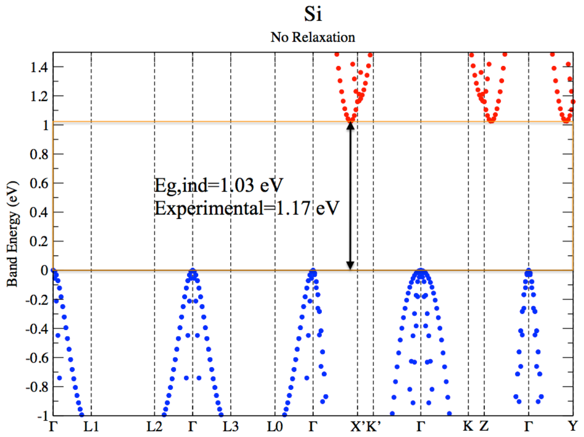
- DFT packages such as VASP, Abinit, Quantum-Espresso are routinely used to predict the properties of new materials, and are used to provide motivation for experimental demonstration of such materials.

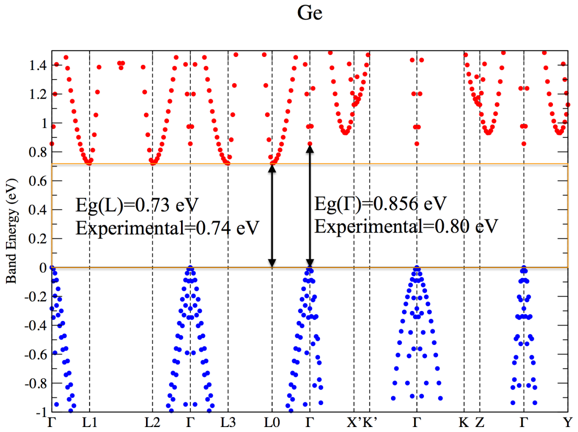
- Accuracy of DFT depends on Exchange & Correlation potential (Vxc):
  F. Tran, P. Blaha (MBJLDA), DOI: 10.1103/PhysRevLett.102.226401:
  “Accurate Band Gaps of Semiconductors and Insulators with a Semilocal Exchange-Correlation Potential”.



Ab-Initio Simulations and Accuracy

- Accuracy of DFT simulations of Si, Ge, $Si_{1-y}C_y$ alloys strained to Si, provides credibility for SLs.





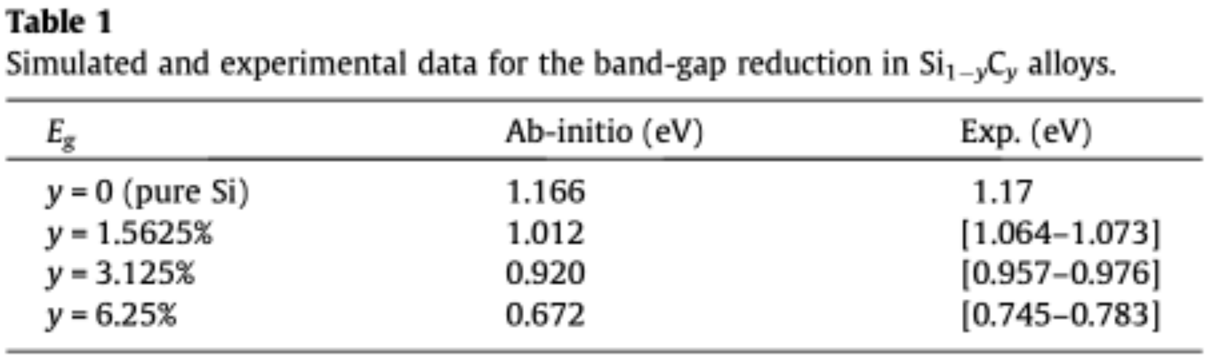


Table 1

Simulated and experimental data for the band-gap reduction in $Si_{1-y}C_y$ alloys.

E_g	Ab-initio (eV)	Exp. (eV)
$y = 0$ (pure Si)	1.166	1.17
$y = 1.5625\%$	1.012	[1.064–1.073]
$y = 3.125\%$	0.920	[0.957–0.976]
$y = 6.25\%$	0.672	[0.745–0.783]

- The exact same material composition epitaxially strained to different crystallographic orientations can lead to very different Band Structures, Band Offsets and optoelectronic properties.
- Substrates with multiple crystallographic orientations were demonstrated in the mid-2000's through different methods. See for example: M. Yang et al., "Hybrid-orientation technology (HOT): Opportunities and challenges". IEEE Trans. Electr. Dev., vol. 53, pages 965-978, 2006; DOI: 10.1109/TED.2006.872693.

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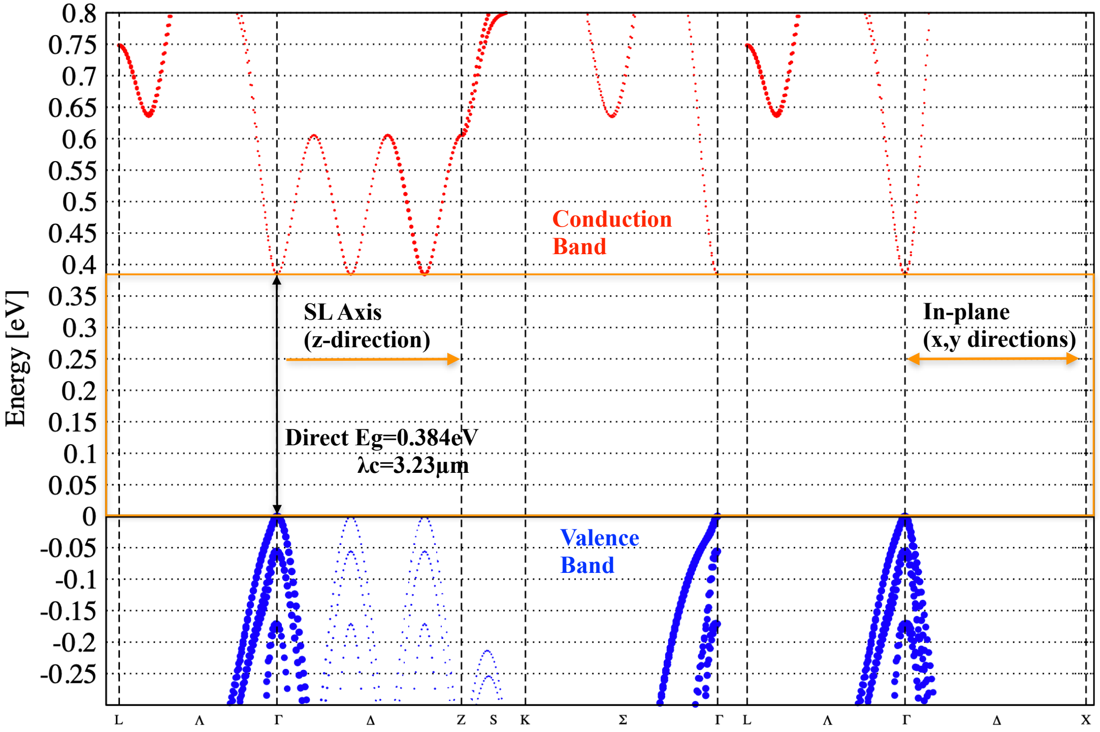
Ab-Initio Results for Group-IV SLs in the SWIR

Direct band-gaps in the Infra-Red

An example of a Si-Ge-C SL, strain-balanced to Si, with a direct band-gap that can capture SWIR up to the 3.2µm wavelength with high efficiency.

Si-Ge-C SL#1 on Si (0 0 1): DFT Band Structure Calculation

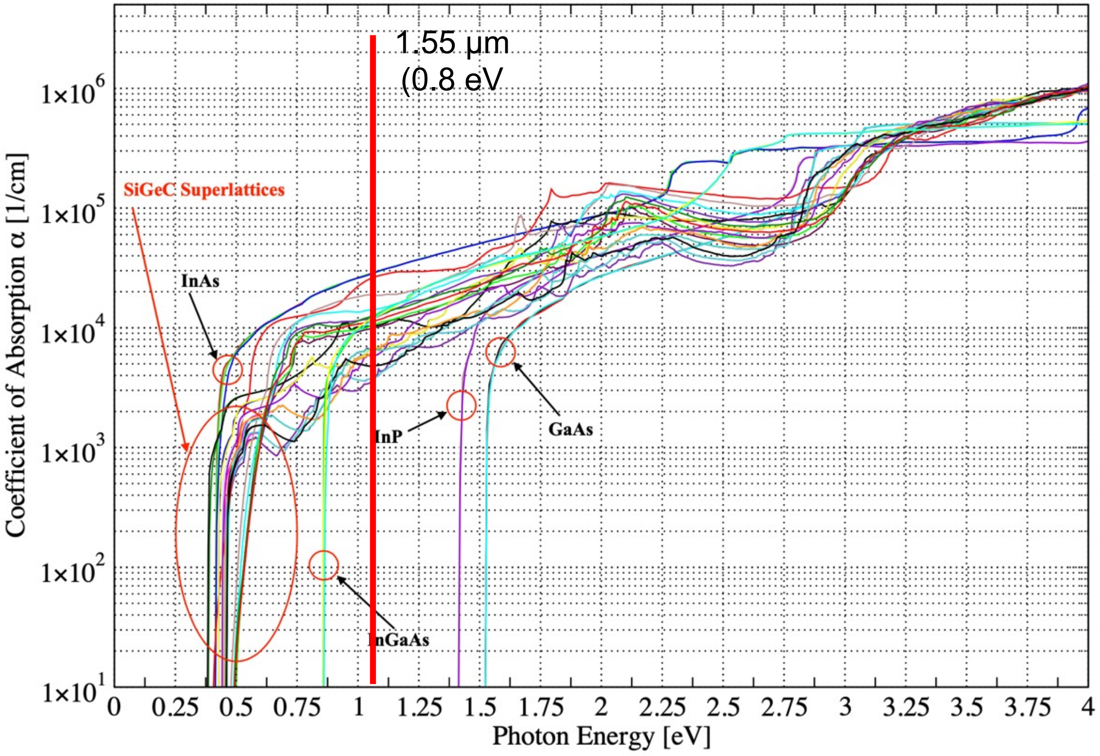


Better photo-absorption than III/V materials:

Simulation results for Si-Ge-C superlattices and III-V materials show high coefficient of absorption for superlattices over a wider range in IR than III-V materials.

SiGeC SLs strained to Si(0 0 1) & Reference III-V materials

SiGeC SLs: $E_G = 0.384 \dashrightarrow 0.462$ [eV] or $\lambda_C = 3.229 \dashrightarrow 2.683$ [µm]



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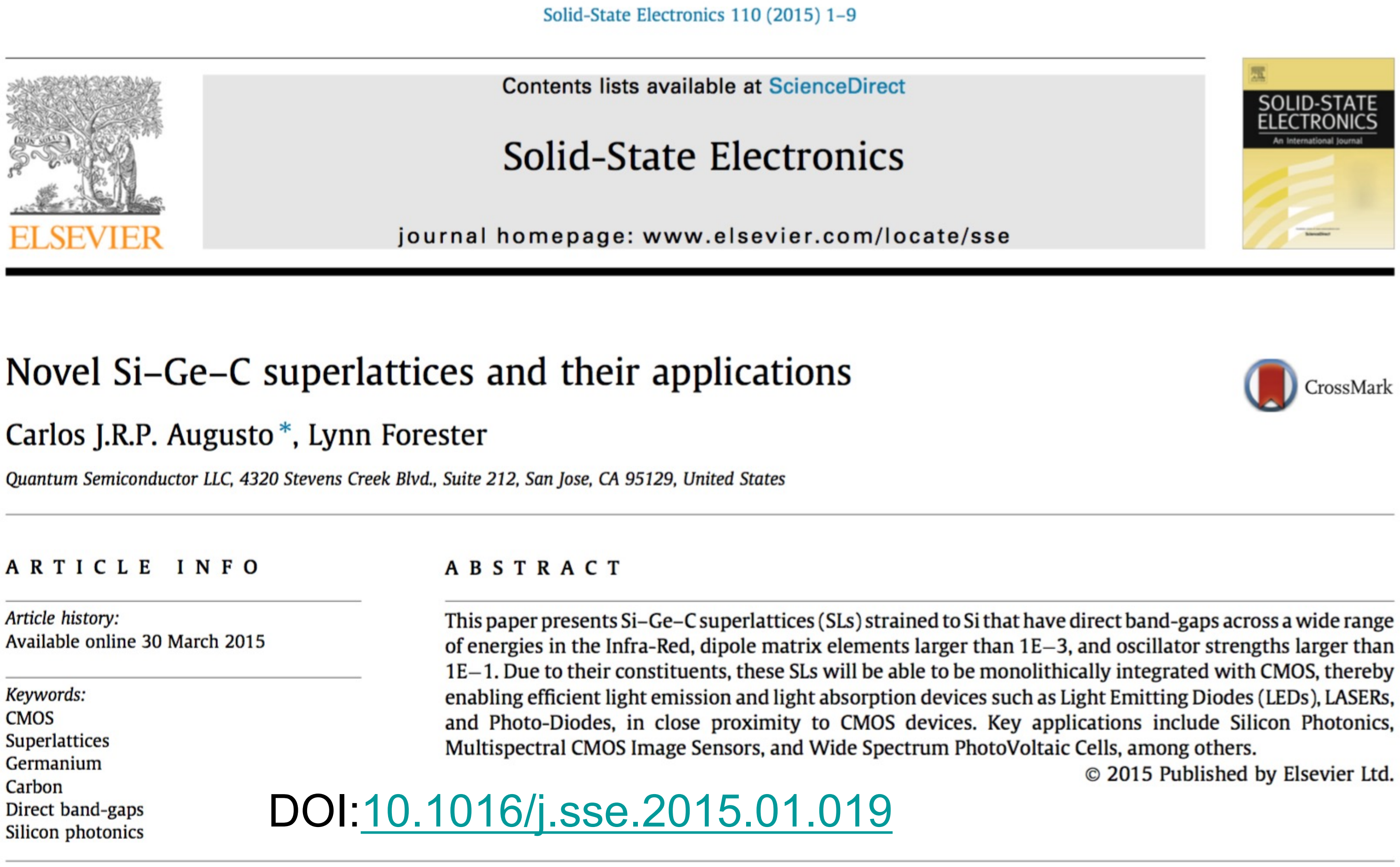
Group-IV Si-Ge-C Superlattices with Direct Band-Gaps

Proceedings Paper of Invited Talk at ISTDM 2014 (Singapore)

First public presentation on reporting the discovery of Si-Ge-C Superlattices with Direct Band-Gaps.

Describes physical insight and credibility of ab-initio (DFT) simulations.

Simulations of SL compositions with some layers having 20% Carbon.



Solid-State Electronics 110 (2015) 1–9

Contents lists available at ScienceDirect

Solid-State Electronics

journal homepage: www.elsevier.com/locate/sse

Novel Si–Ge–C superlattices and their applications

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ARTICLE INFO

Article history:
Available online 30 March 2015

Keywords:
CMOS
Superlattices
Germanium
Carbon
Direct band-gaps
Silicon photonics

ABSTRACT

This paper presents Si–Ge–C superlattices (SLs) strained to Si that have direct band-gaps across a wide range of energies in the Infra-Red, dipole matrix elements larger than 1E−3, and oscillator strengths larger than 1E−1. Due to their constituents, these SLs will be able to be monolithically integrated with CMOS, thereby enabling efficient light emission and light absorption devices such as Light Emitting Diodes (LEDs), LASERs, and Photo-Diodes, in close proximity to CMOS devices. Key applications include Silicon Photonics, Multispectral CMOS Image Sensors, and Wide Spectrum PhotoVoltaic Cells, among others.

DOI:10.1016/j.sse.2015.01.019

Group-IV SLs: for Analog & Quantum Photonics

Unique Optoelectronic Properties in select Superlattices

Some SLs are Non-Centrosymmetric Crystals:

- Pockels Effect: enables Electro-Optical Phase Modulators.
- Photo-Galvanic Effect: photo-voltages larger than band-gaps.

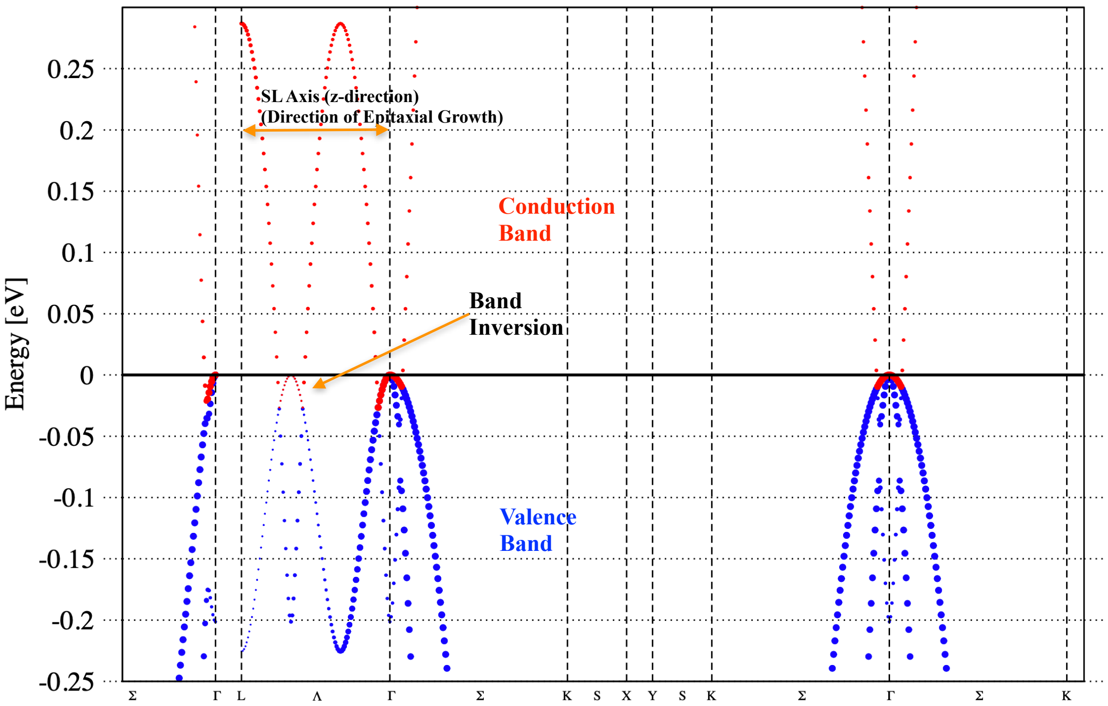
Some SLs have Topological Band-Structures:

- Band inversion at Γ-point and along SL axis.
- Nonlinear enhancements of optoelectronic properties.
- Photon frequency multiplication and division which enable frequency combs and entanglement for quantum photonics.
- Enhanced thermoelectric properties for energy harvesting.

3D Topological Insulators & Semimetals:

- Topological SLs: can be building blocks of devices for Quantum Photonics.
- Quantum Photonics: Room Temperature operation of Quantum-Computing, - Sensing, - Communications.

Si-Ge-C SL#2 on Si (1 1 1): DFT Band Structure Calculation



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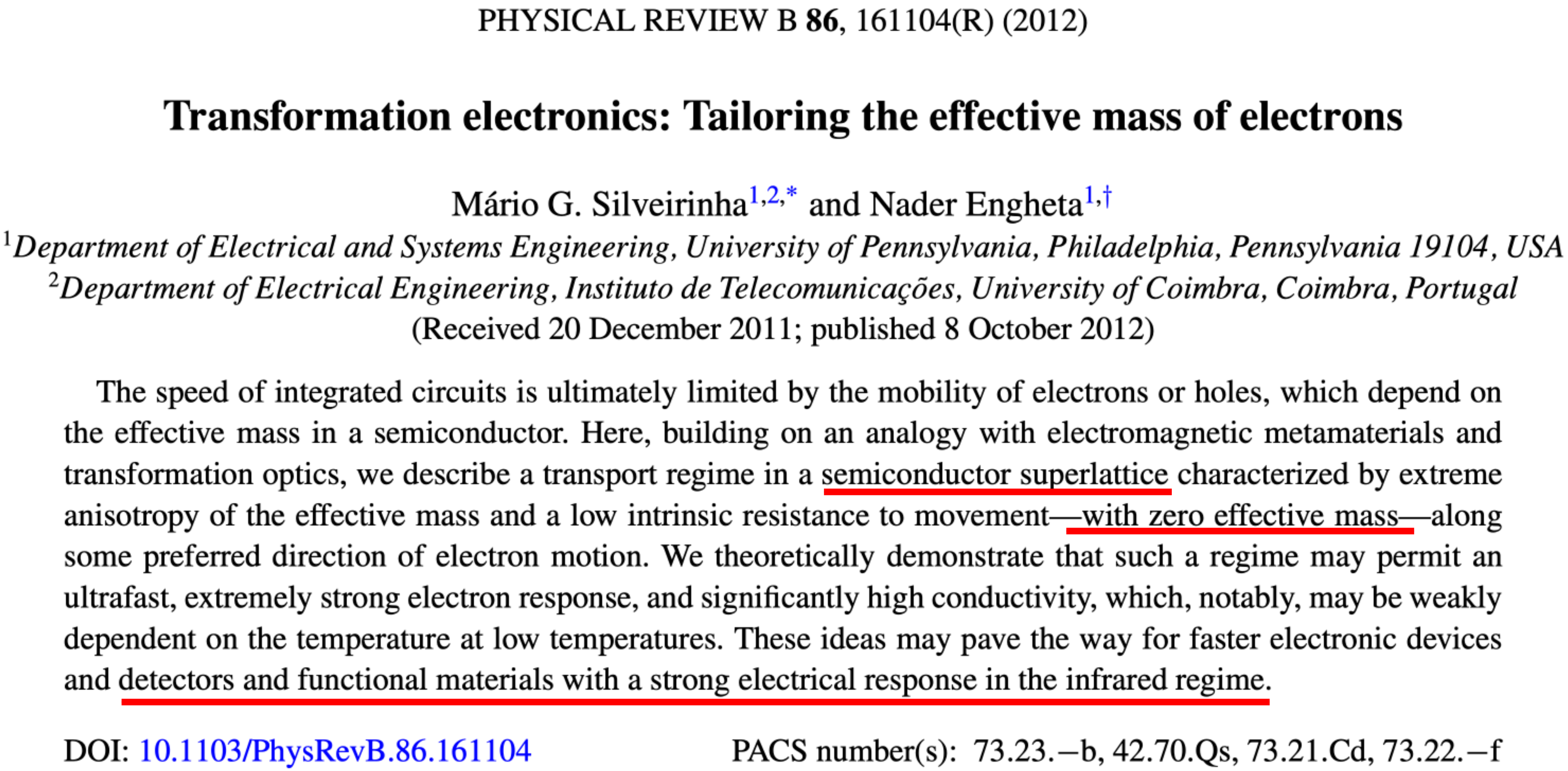
SLs: The Promise of Ideal Transport Properties

Theoretical prediction of zero mass along SL axis and infinite mass for in-plane directions



PHYSICAL REVIEW B **86**, 161104(R) (2012)

Transformation electronics: Tailoring the effective mass of electrons

Mário G. Silveirinha[1,2,*] and Nader Engheta[1,†]
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(Received 20 December 2011; published 8 October 2012)

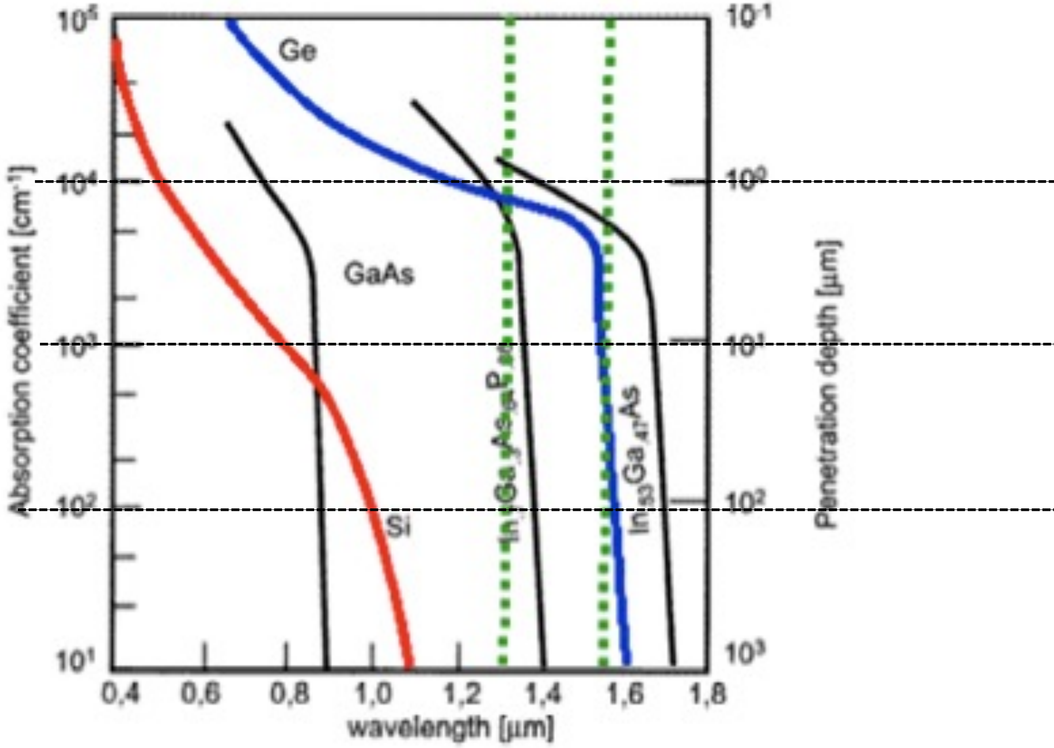
The speed of integrated circuits is ultimately limited by the mobility of electrons or holes, which depend on the effective mass in a semiconductor. Here, building on an analogy with electromagnetic metamaterials and transformation optics, we describe a transport regime in a semiconductor superlattice characterized by extreme anisotropy of the effective mass and a low intrinsic resistance to movement—with zero effective mass—along some preferred direction of electron motion. We theoretically demonstrate that such a regime may permit an ultrafast, extremely strong electron response, and significantly high conductivity, which, notably, may be weakly dependent on the temperature at low temperatures. These ideas may pave the way for faster electronic devices and detectors and functional materials with a strong electrical response in the infrared regime.

DOI: 10.1103/PhysRevB.86.161104 PACS number(s): 73.23.−b, 42.70.Qs, 73.21.Cd, 73.22.−f

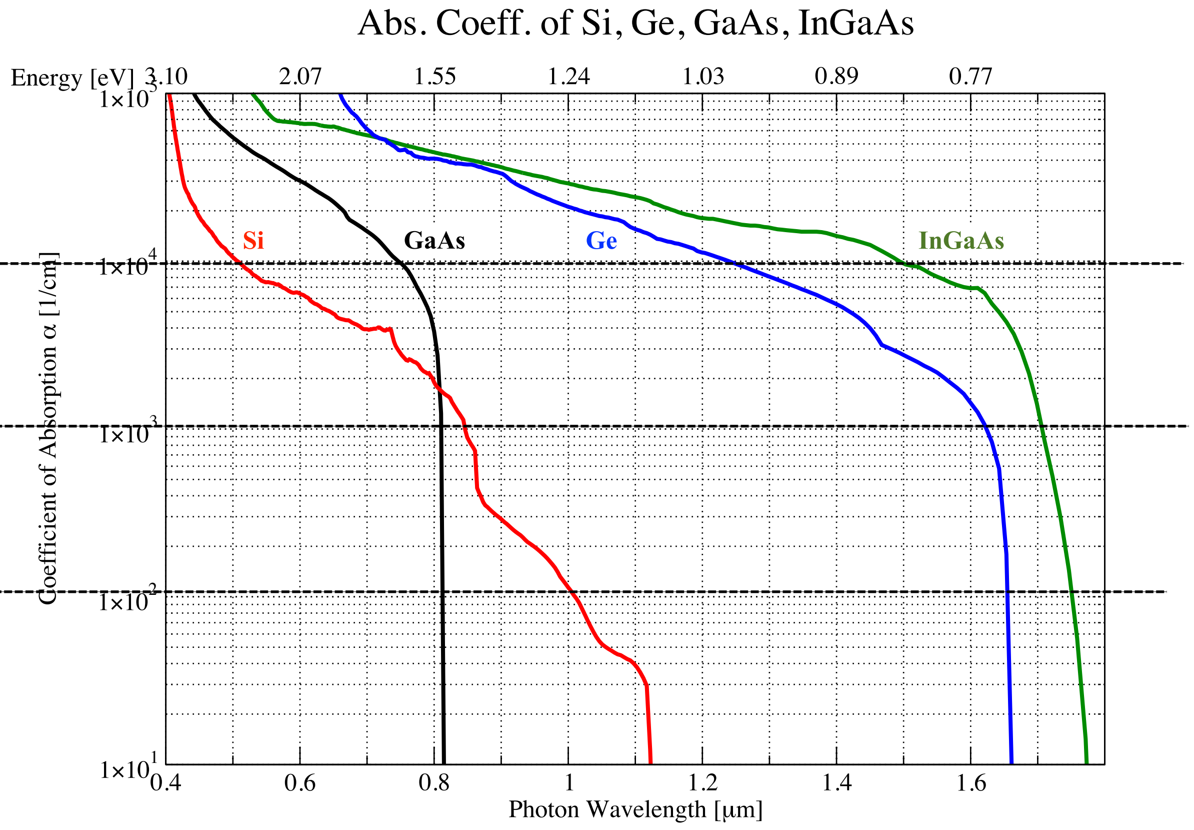
Coefficient of Absorption of Si, Ge, & Superlattices

Comparison of Coefficient of Absorption from Experiments & Ab-Initio Calculations

Experimental data from textbooks



Calculations Ab-Initio



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Quantum Efficiency for Si, Ge, InGaAs, Group-IV SL

Collaboration with Silvaco

Calculations with Silvaco's ATLAS Device Simulator (with customized features)

Device type: P-I-N Photodiode

Dimensions: (1x1x1) μm^3 for all materials

High doping only at the top and bottom in the vertical direction.

Ideal ohmic contacts

Si - Standard models.

SL - Approximations:

- Ab-Initio Effective Mass
- Mobility proportional to Si (ratio of masses)
- Ab-Initio Abs. Coeff.
- Density of defects for SRH & Auger recombination same as for Si.

InGaAs - Sotoodeh mobility model (Caughey-Thomas parametrization for III-V) https://doi.org/10.1063/1.372274

Ge - Constant mobilities mun=3900 and mup=1900 cm2/Vs (default Atlas values for Ge). B=0.178E-13cm3/s

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Quantum Efficiency for Si, Ge, InGaAs, Group-IV SL

Band-gaps [eV]

Si (Ind.) = 1.12

Ge (Ind.) = 0.66

$In_{0.53}Ga_{0.47}As$ (Dir.): 0.74

SL (Dir.) = 0.38

Wavelength cutoff [µm]:

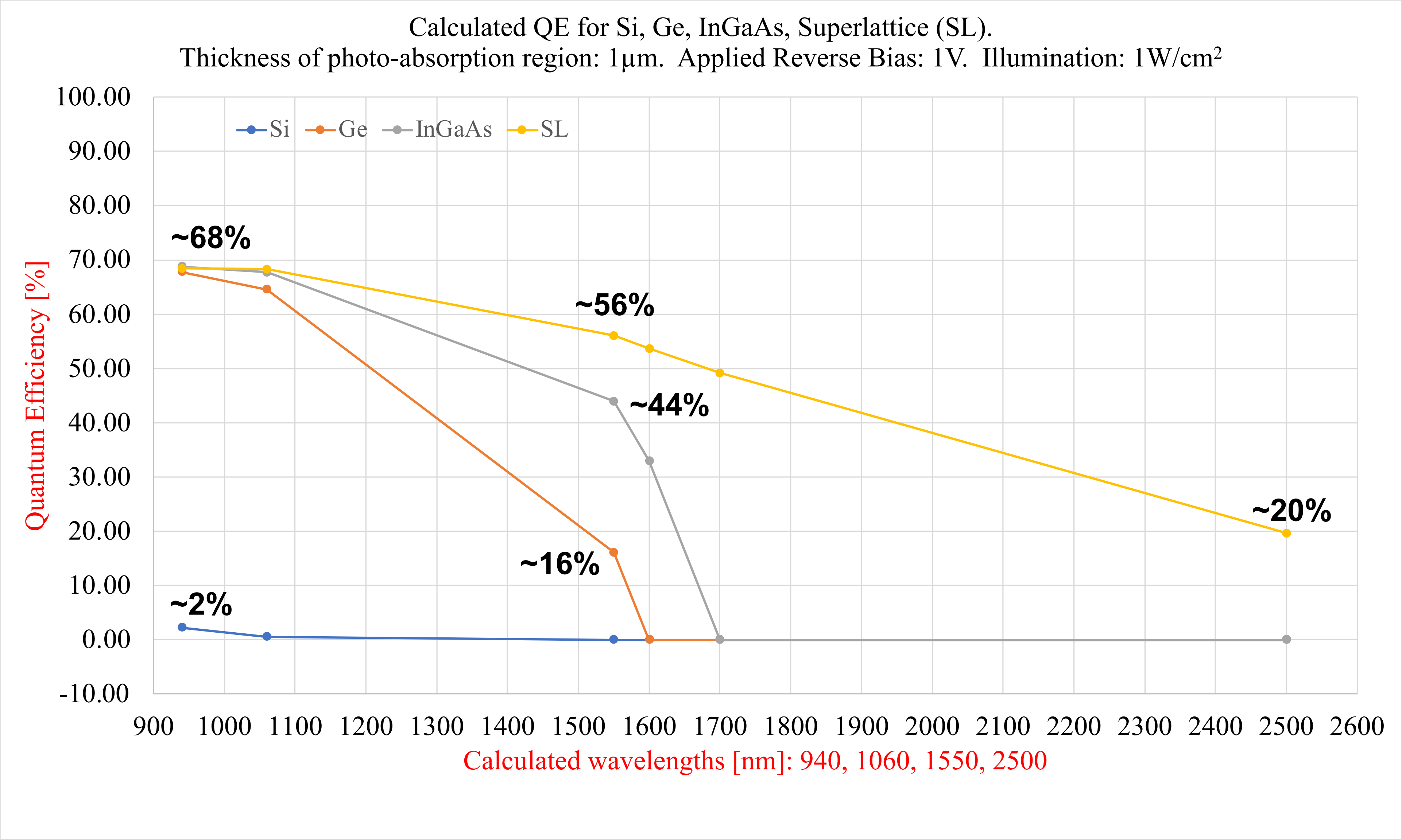
Si = ~1.1

Ge = ~1.8

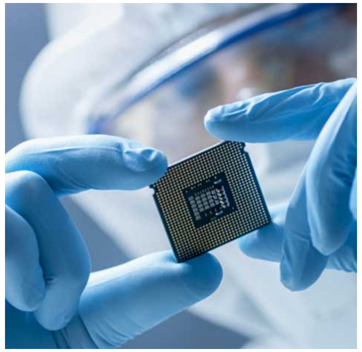
$In_{0.53}Ga_{0.47}As$ = ~1.7

SL: ~ 3.23

QE can be further increased with thicker absorption regions.

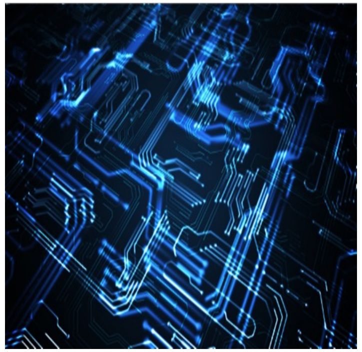


Revolution in Materials Advancing Many Applications

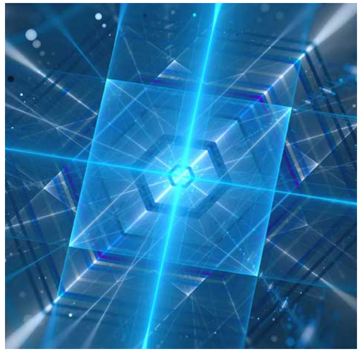


Sensors and Detectors

Silicon Photonics



AI and Data Center HPC



Quantum Photonics

Single Chip LiDAR / ADAS

5G & 6G Data Comm

Silicon Photovoltaics

Cybersecurity

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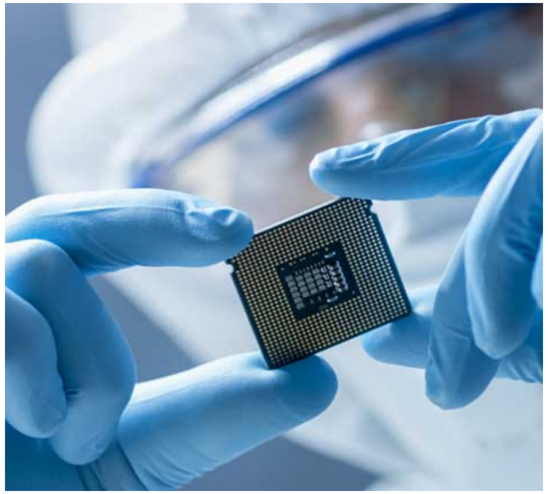
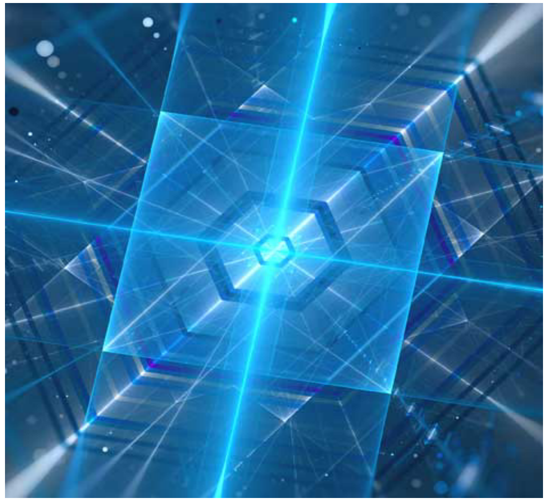
Thank you and Summary

New Materials for Infrared Absorption & Emission monolithically-integrated with CMOS



Lasers and Photodiodes side-by-side in one chip



New capabilities impacting multiple markets: Photonics, Imaging, AI, HPC, Quantum computing, LiDAR, AR/VR.

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