MATERIALS FOR THE GREEN ENERGY TRANSITION

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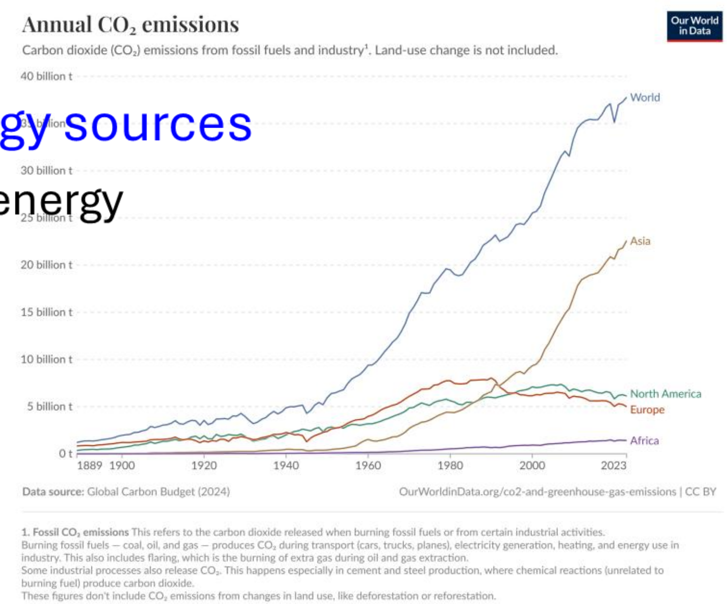
Two main challenges

- We are constantly using the Earth's resources
  - Shift away from scarce materials
  - Materials must be recycled
- Climate challenges – sustainable energy sources
  - The Earth's current and predicted use of energy
  - Sustainable sources
  - Energy storage
  - Power-to-X



Solar energy

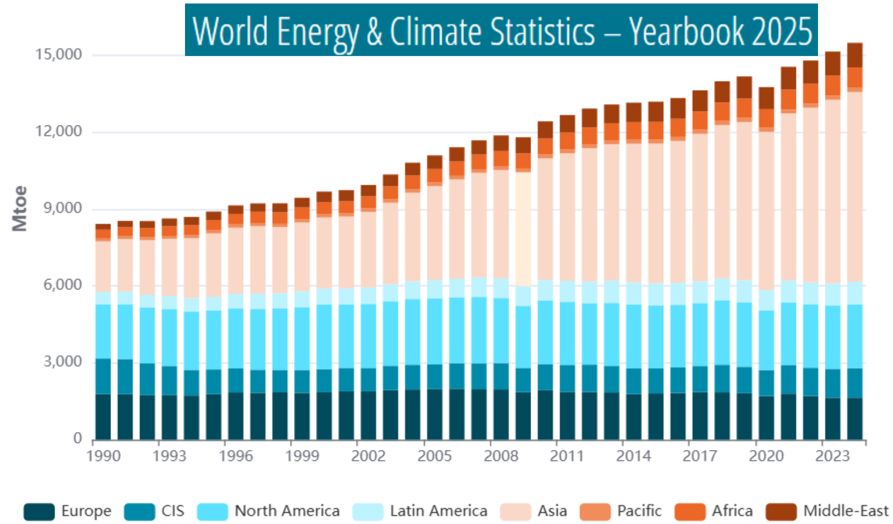
- Global annual energy consumption 2023

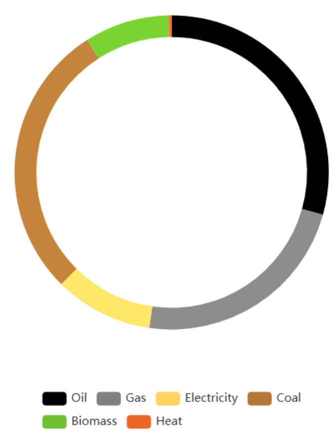
  620×10^{18} joules, 170×10^{17} watt hours

- Solar radiation: 1 kW/m²
  - X (8x365 hours)x15% =500 kW hours/m²/year
  - $170 \times 10^{17} / 500 \times 10^{3} = 3.4 \times 10^{11}$ m² =340,000 km²
  - The area of Germany

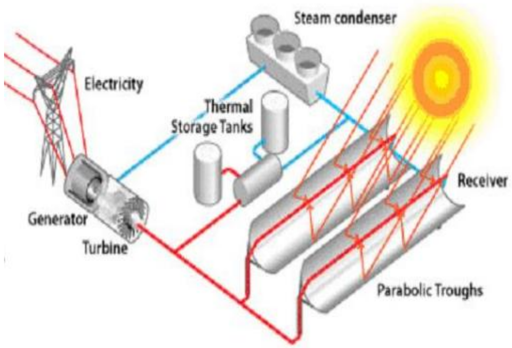
- PV cells
  - What limits the efficiency?

- What limits the use of solar energy
  - **Storage**
  - **Prize**

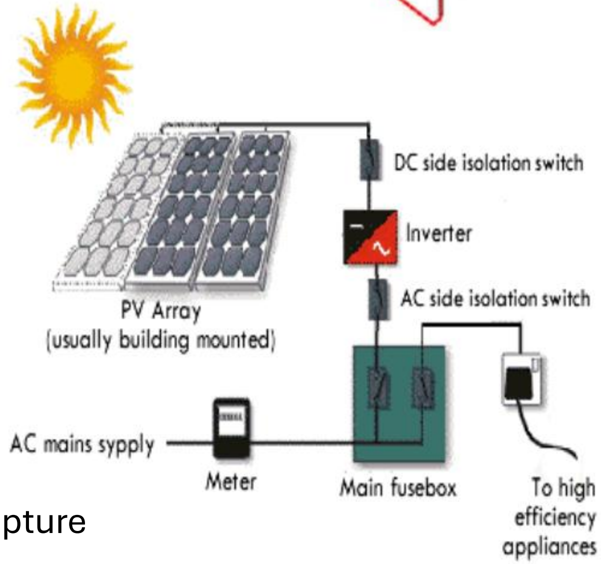




Solar energy

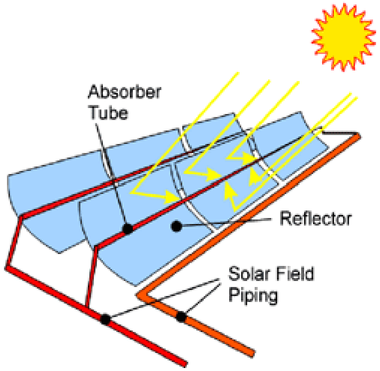


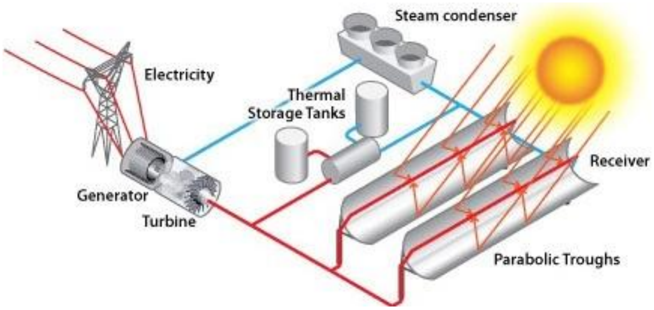
- Thermal energy
  - Solar radiation to heat
  - Concentrator systems
  - Absorber tubes – high temperature coatings
  - Solar radiation → Heat → Steam → Electricity
  - Solar thermo-electric
- PV (Photo Voltaic) cells
  - Generation 1: single Si diode cells
  - Generation 2: thin films cells
  - Generation 3: multijunction cels
- Solar driven catalysis
  - Photocatalysis
  - PhotoElectroCatalysis (PEC)
  - Energy generation and storage, chemical processes, CO_2 capture



Cu International Copper Association Copper Alliance

Concentrated Solar Power (CSP) systems





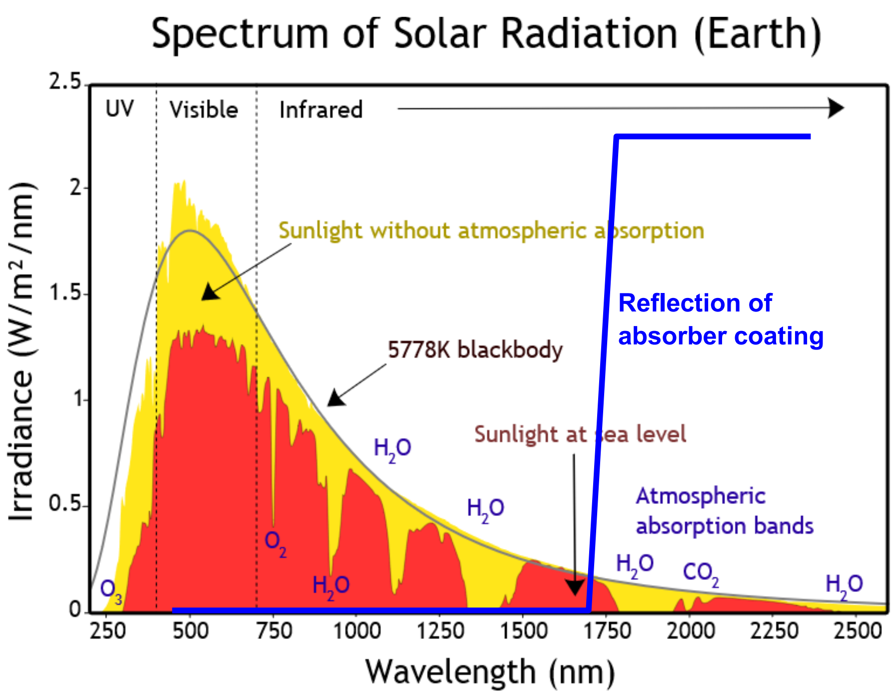
Hot liquid for:

Direct heating

Steam generation

Parabolic Trough Concentrating Solar Collector at Kramer Junction, California

Adjusting coating to solar spectrum



Ideal coating

- highly absorbing over the visible and near-infrared covering the major part of the solar spectrum
- reflecting in the infrared region to suppress thermal radiation from the heated absorber
- stable at elevated temperatures
- fabricated through simple deposition techniques

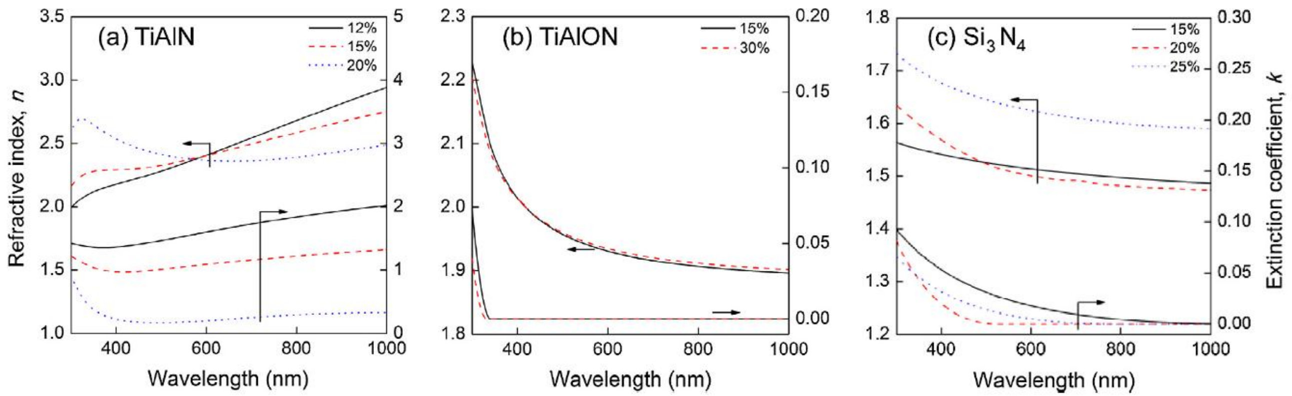
Nitrides and oxy-nitrides

Thermally stable

Adjustable properties

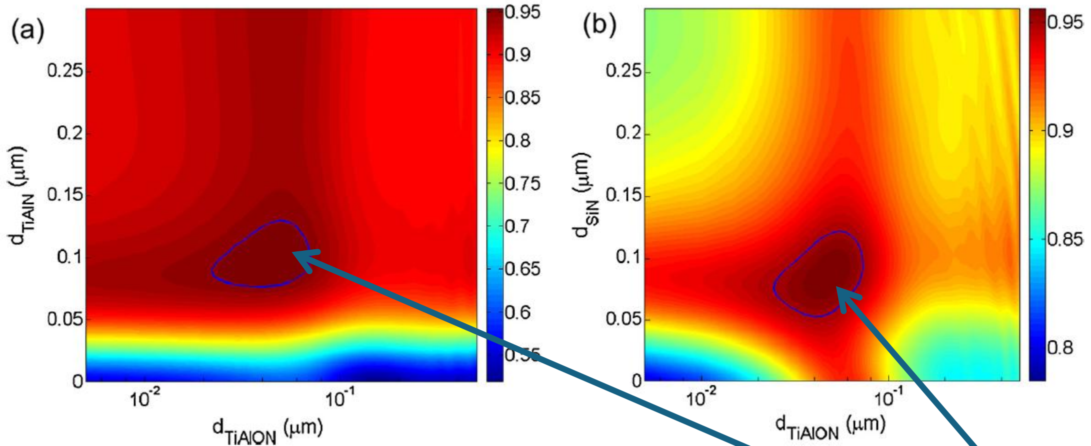
Absorber stack

- Optically thick Mo layer at the bottom (IR reflection)
- Decreasing extinction towards the top
- Antireflection layer thicknesses
- Dependence on Nitrogen content



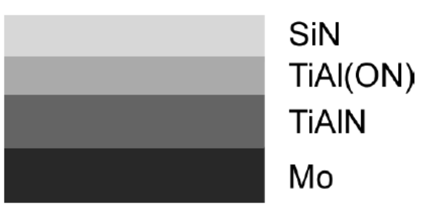
Stacks must be developed together with machine

Optimization of layer thicknesses

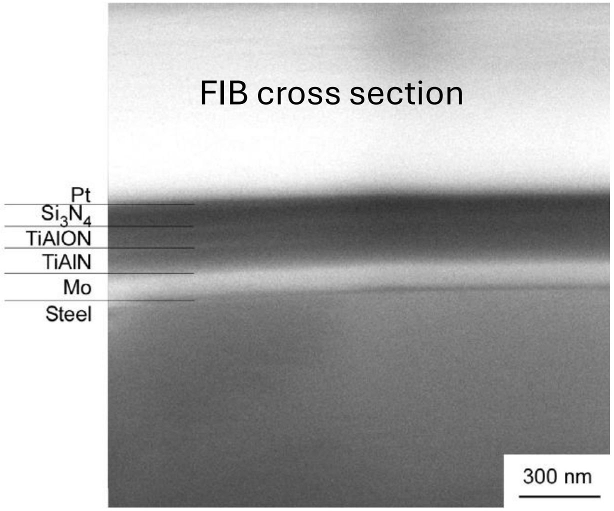


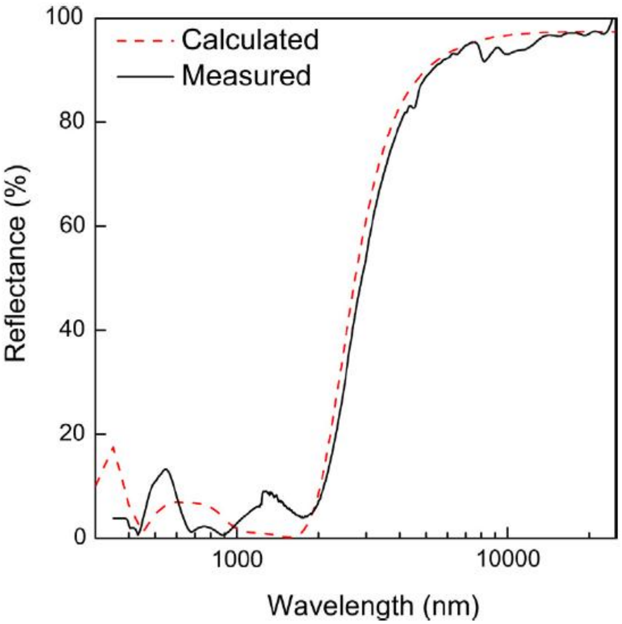
- **Absorptance** as a function of layer thicknesses
- Regions with absorptance > 95% marked
- Reasonable production tolerance
- Layer thicknesses:
  - Mo: 100 nm
  - TiAlN: 80-120 nm
  - TiAlON: 50 nm
  - Si_3N_4: 100 nm

Production tolerance



Experimental stack



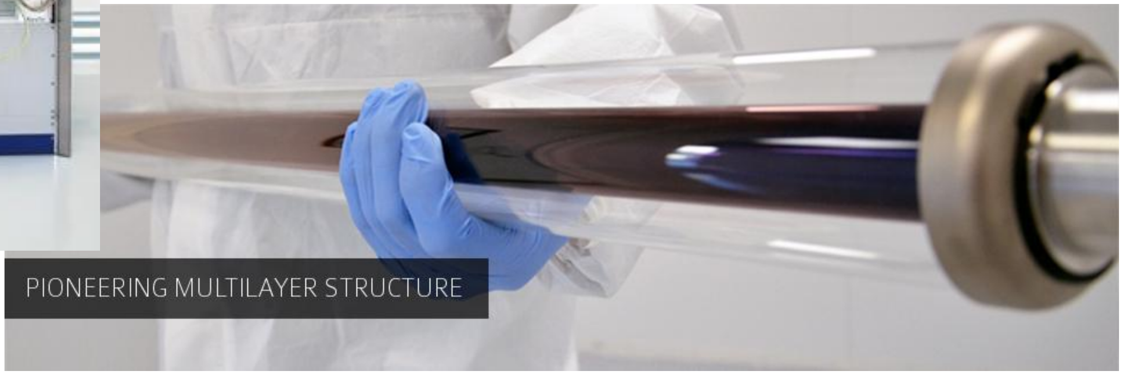


- Solar absorption: 94.5%
- Thermal emission: 5.2% @ 125 C,   12.8% @ 375 C

Solar Energy, **118**, 410-418 (2015)

PolyCSP Aps

Company formed to develop and produce absorber tubes



What limits the efficiency of solar cells

Photon flux from Sun: $$n_{sun}(E) = \frac{2\pi E^2}{h^3c^2} \cdot \frac{1}{e^{E/kT_{sun}} - 1}$$

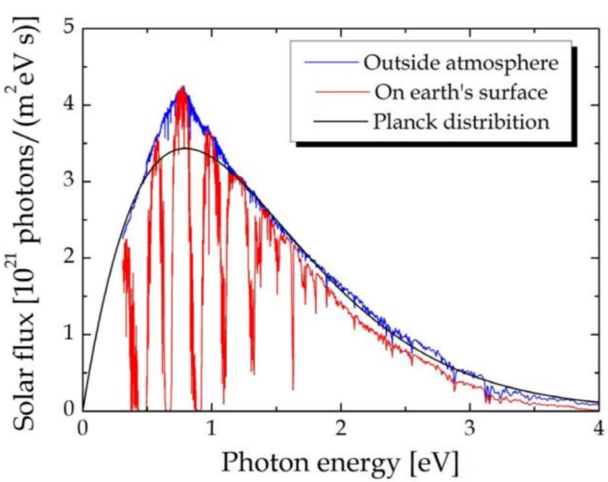
T_{sun} = 5800 K, $k_B T_{sun}$ = 0.5 eV

Photon flux at Earth: $$n_E^{(0)}(E) = n_{sun}(E)\frac{R_{sun}^2}{R_E^2}$$:

R_{Sun}: Radius of Sun
R_E : Distance to Earth

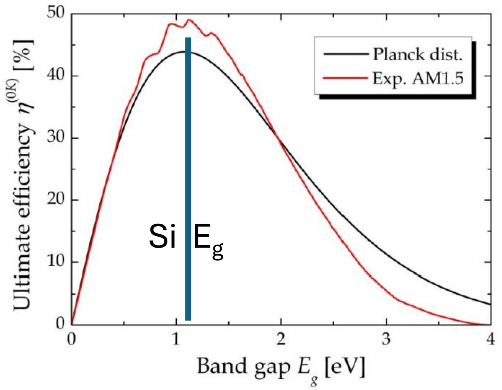
Intensity: $$I_E^{(0)} = \int_0^\infty n_E^{(0)}(E) E dE = \frac{R_{sun}^2}{R_E^2} \cdot \frac{2\pi^5 (kT_{sun})^4}{15 h^3 c^2}$$

Thomes Garm Pedersen



~ 1000 W/m^2 at Earth surface

Solar cell efficiency

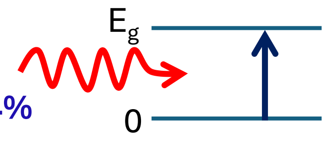


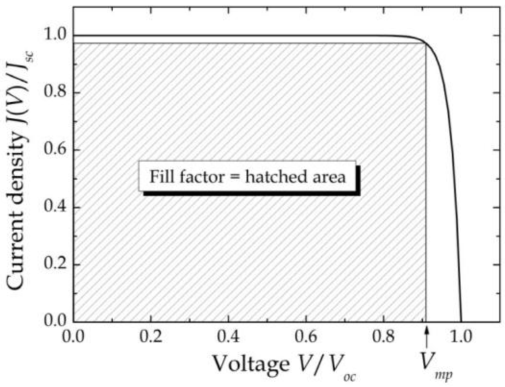
Ultimate efficiency

$$\eta^{(0K)} = E_g \int_{E_g}^{\infty} n_E(E)dE \Big/ \int_0^{\infty} n_E(E)E\,dE$$

Si good for PV !

Max ideal efficiency 44%



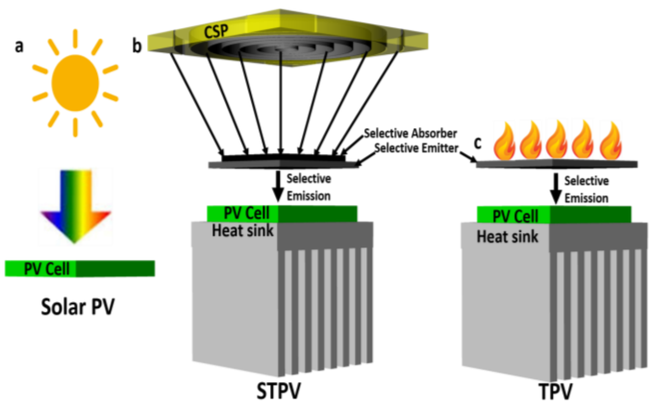


Shockley – Queisser Limit:

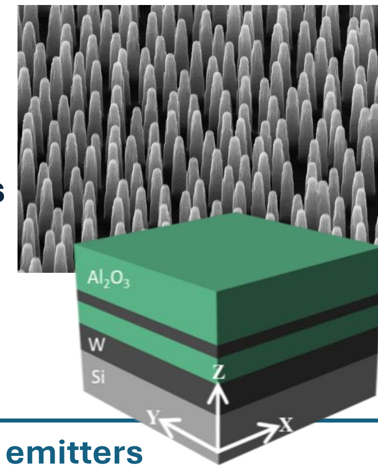
Thermal radiation and electron recombinations

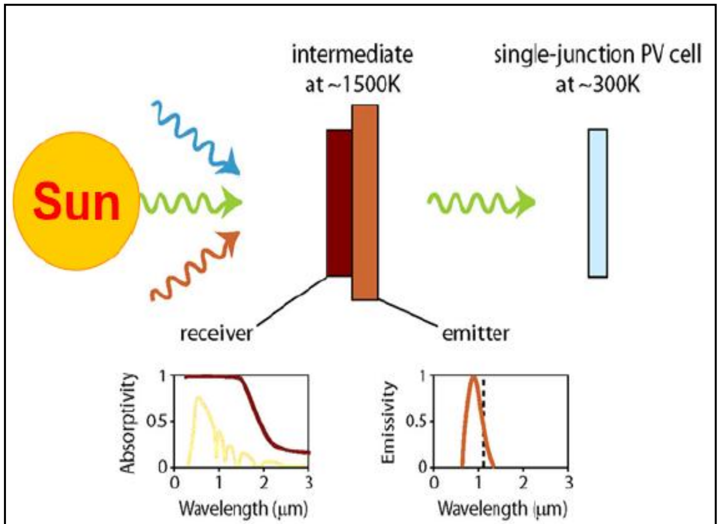
Single pn-junction Si cell: **Max efficiency 33%**

Solar and heat radiation to electricity
ThermoPhotoVoltaics



Design of Abs/Emis: Nanostructures and thin film stacks





Design of **absorbers and emitters**
Emission only at band gap of PV cell
May break the Shockley-Quaisser limit of ~33% for PV cells.

$$\eta = 1 - {T_{cell}}/{T_{emit}}$$ Ideally ~80%

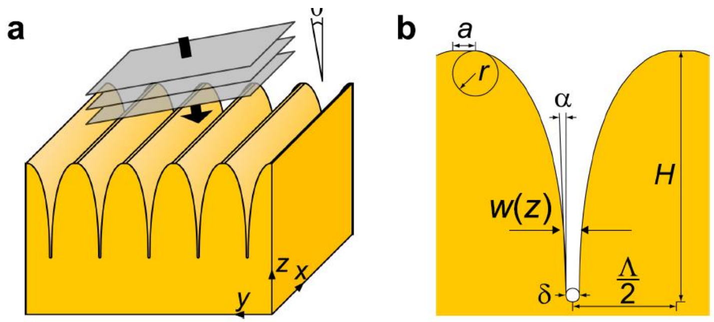
Major challenge: Emis $\propto T^4$ High temp materials!

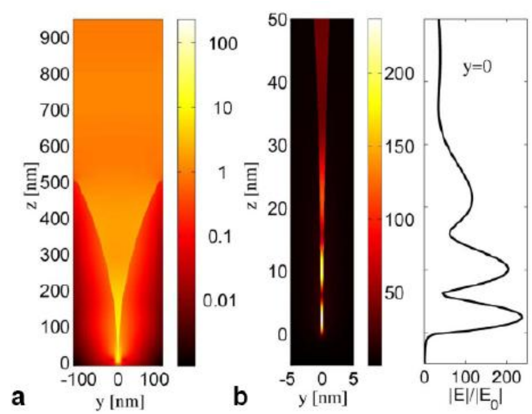
Current record: 29% with 1400 °C emitter
Chirumamilla et al., *Scientific Reports* ***9***, 7241 (2019)

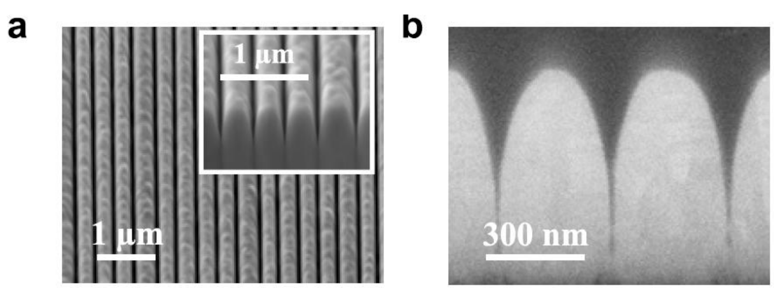
Plasmonic absorbers
Black gold

Nat. Commun. 3, 969 (2012).
https://doi.org/10.1038/ncomms1976

- Structures can be constructed to dissipate almost all optical energy into the surface by excitation of *gap plasmons*



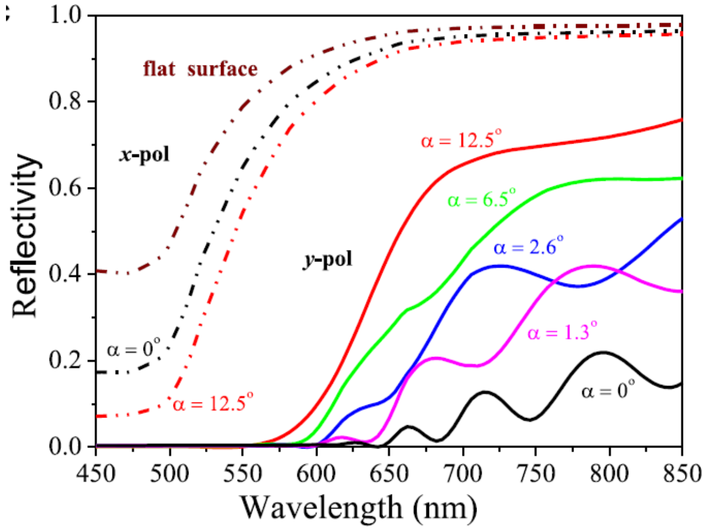




Fabrication by focused ion beam milling

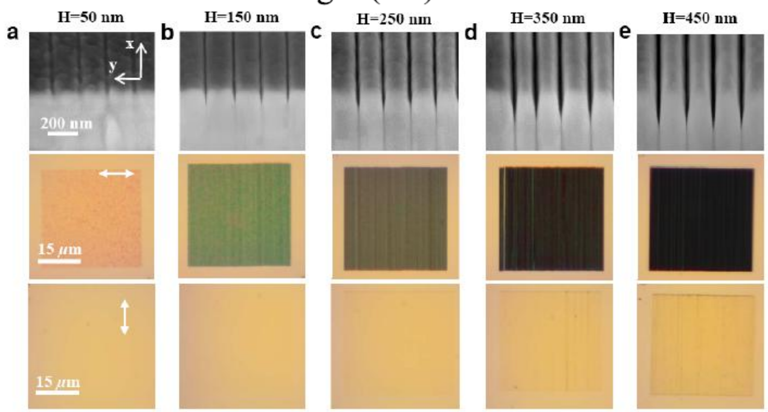
Detailed shape of the grooves very important for the absorption

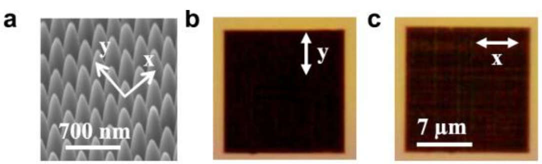
Reflectivity of structures



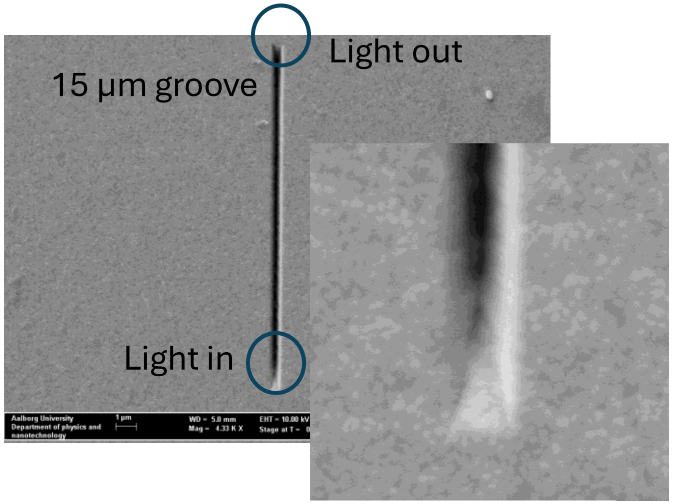
Comparison of flat and structured
Surfaces, different angles of incidence

1D and 2D structures



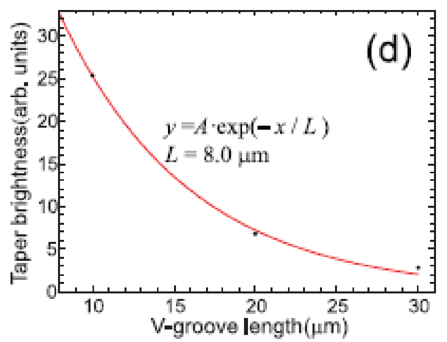


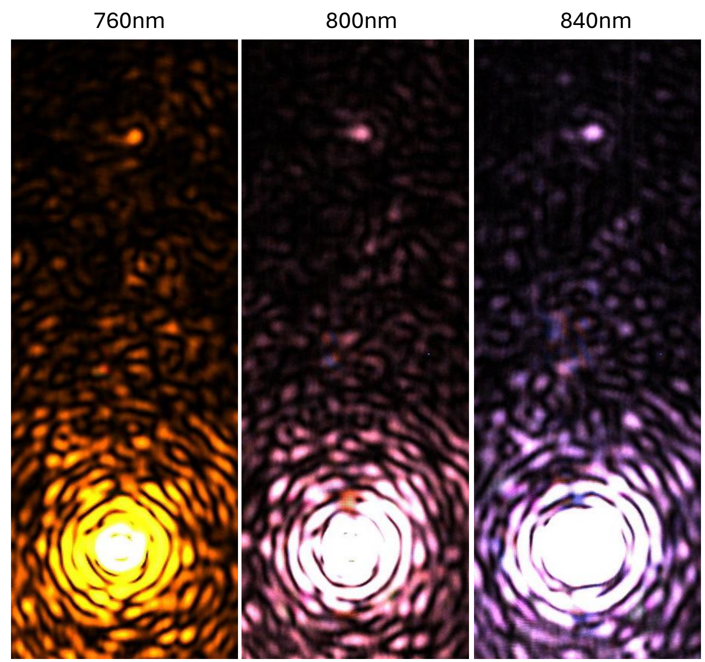
Plasmonic V-groove waveguides



Mirror-like in- and out-coupling

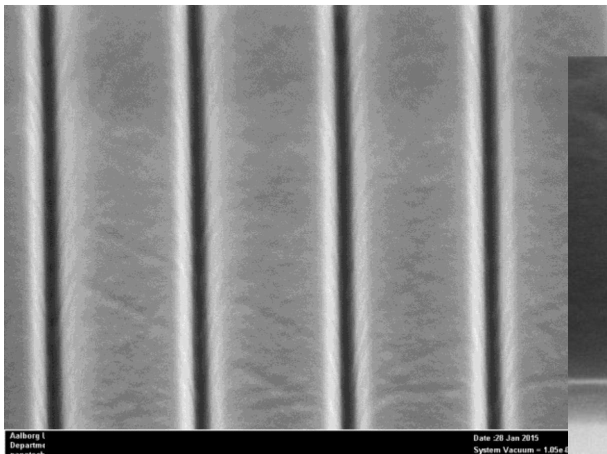
Decay lengths ~8 µm

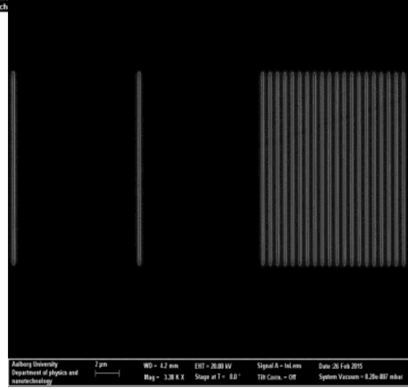


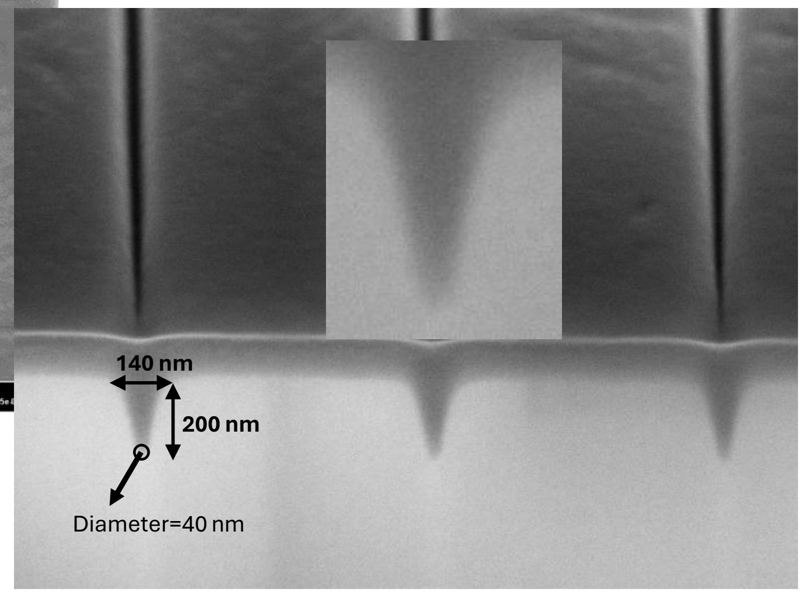


Grooves in Au surfaces – Black Gold

Focused Ion Beam milled structures in Au crystal

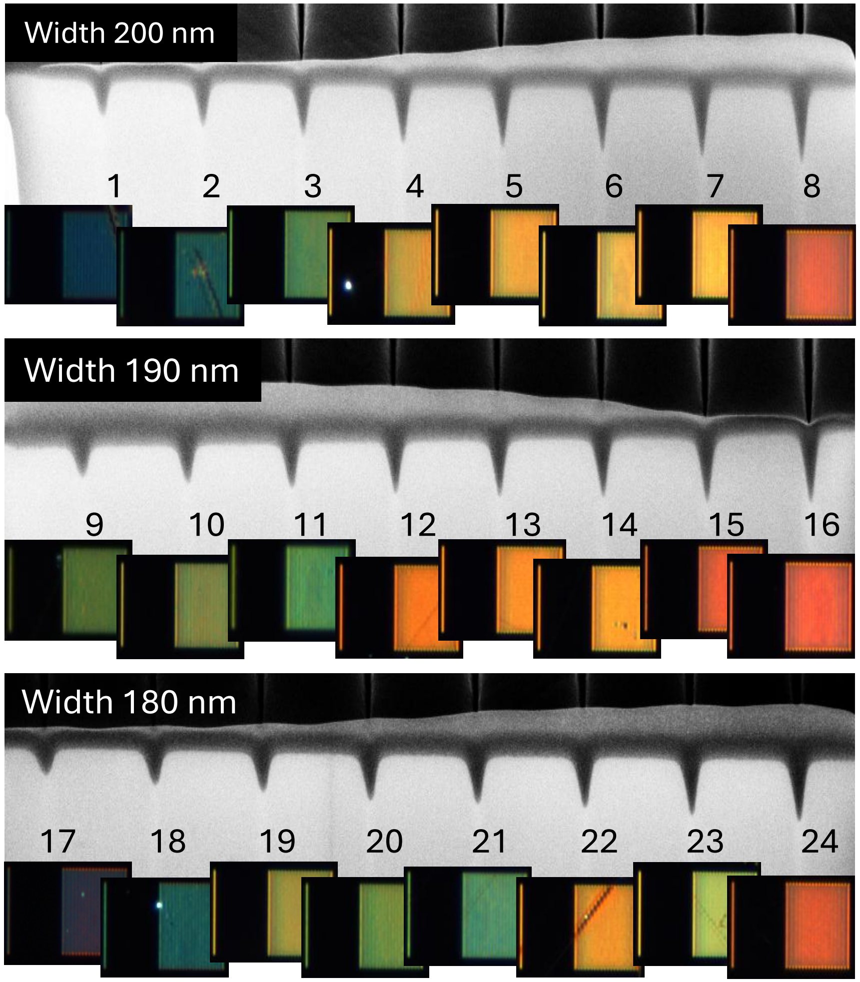






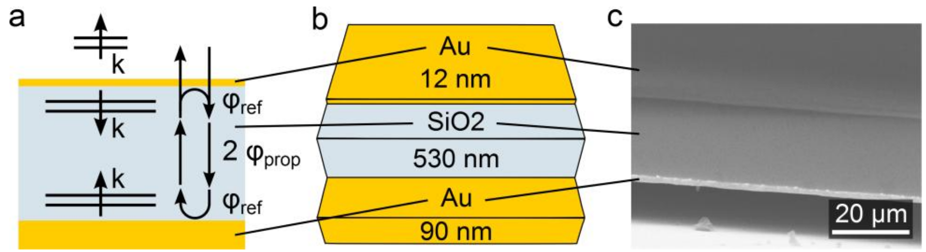
Arrays + single grooves
Expected to work as a gap plasmon resonator

HAR grooves (Ga^+)

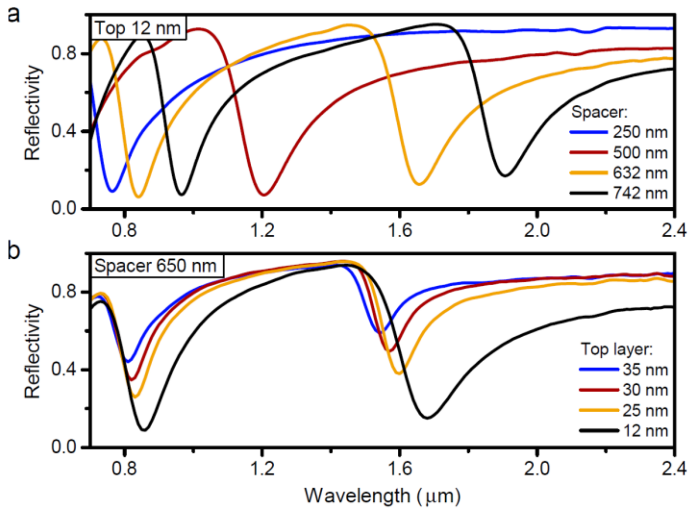


Structure	Width	Depth
1	200	200
2	200	230
3	200	280
4	200	312
5	200	340
6	200	350
7	200	370
8	200	390
9	190	240
10	190	270
11	190	300
12	190	320
13	190	330
14	190	340
15	190	370
16	190	390
17	180	230
18	180	270
19	180	285
20	180	300
21	180	310
22	180	320
23	180	350
24	180	380

Alternative method: Fabry-Perot resonator



Dielectric between two metal layers.
Thin semi transparent top layer.
Thick reflector at bottom.



Absorption dip tunable by thicknes of dielectric layer.

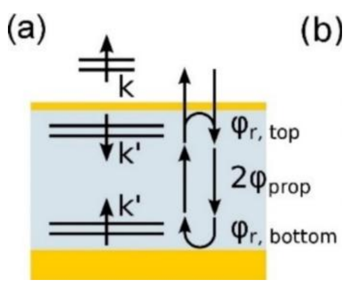
Depth depends on thickness of top layer

Relation between absorption and emission!
Kirchhoff's law

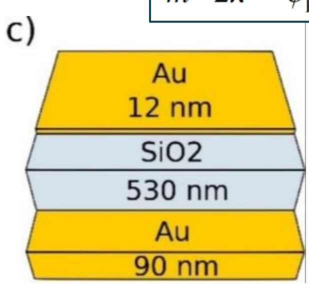
Optics Express Vol. 23, Issue 19, pp. A1111-A1119 (2015)

Near-infrared tailored thermal emission from wafer-scale continuous-film resonators

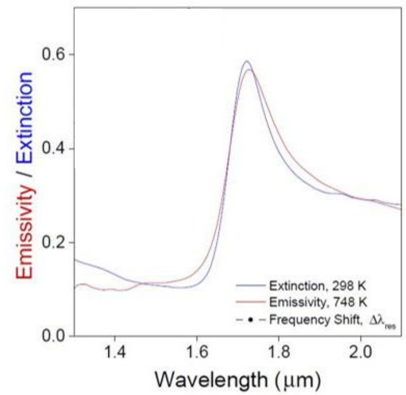
Interference filter



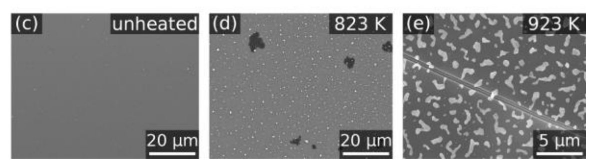
$$m \cdot 2\pi = \phi_{\text{prop.}} + \phi_{\text{r, bottom}} + \phi_{\text{r, top}}$$



Optics Express **23** (2015) A1111



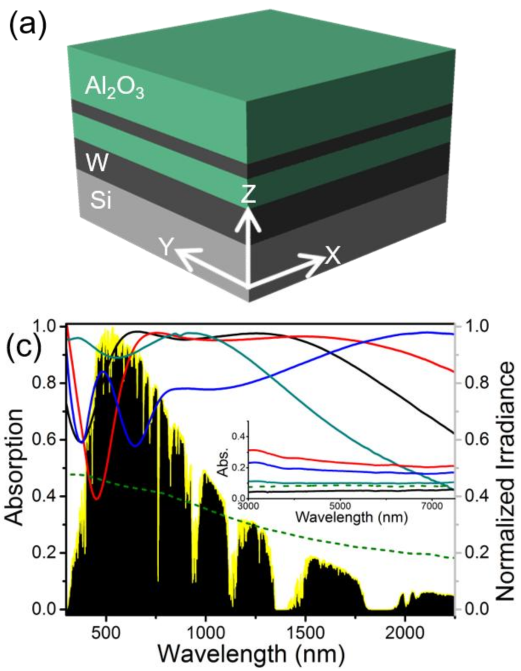
GaSb PV cell: bandgap at 1.7 μm

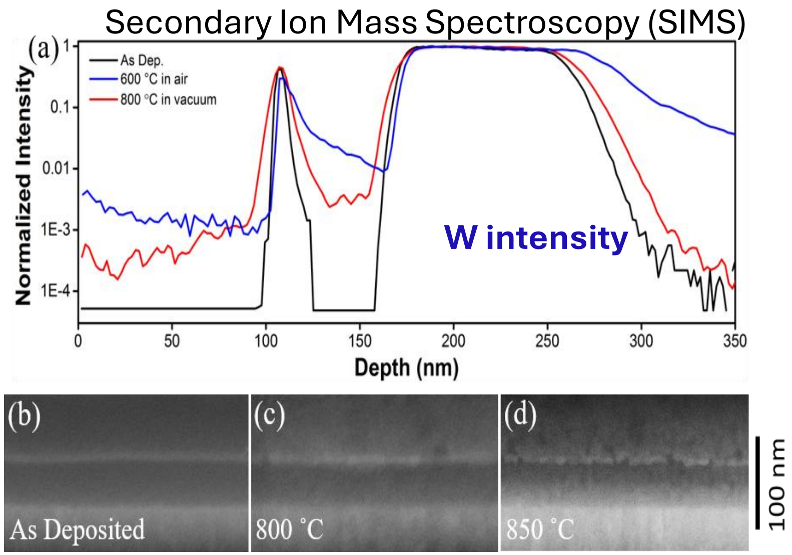


Au films start melting ~ 550^{0}C

Melting point depression

Multilayer tungsten-alumina absorber
Thermal stability





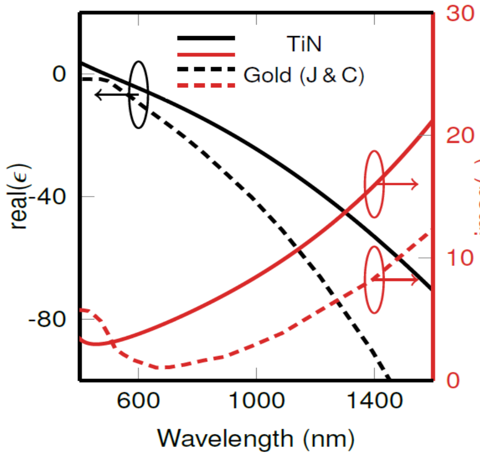
- Metal back reflector
- Partly transparent front reflector
- Dielectric protection layer (also AR coating)
- Absorption controlled by spacer layer thickness

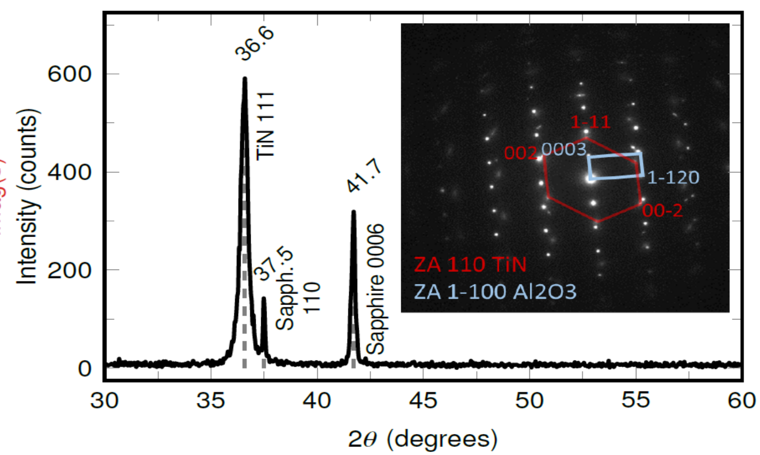
- Thermally stable to 800^{0}C in vaccum
- Diffusion across boundaries and oxidation at higher temperatures

Optical Materials Express **6,** 2704 (2016)

TiN as plasmonic material

Reactive sputter deposition on sapphire at 830^{0}C





(111) TiN ǁ (0001) Al_2O_3

Plasmons: require negative real part of dielectric constant

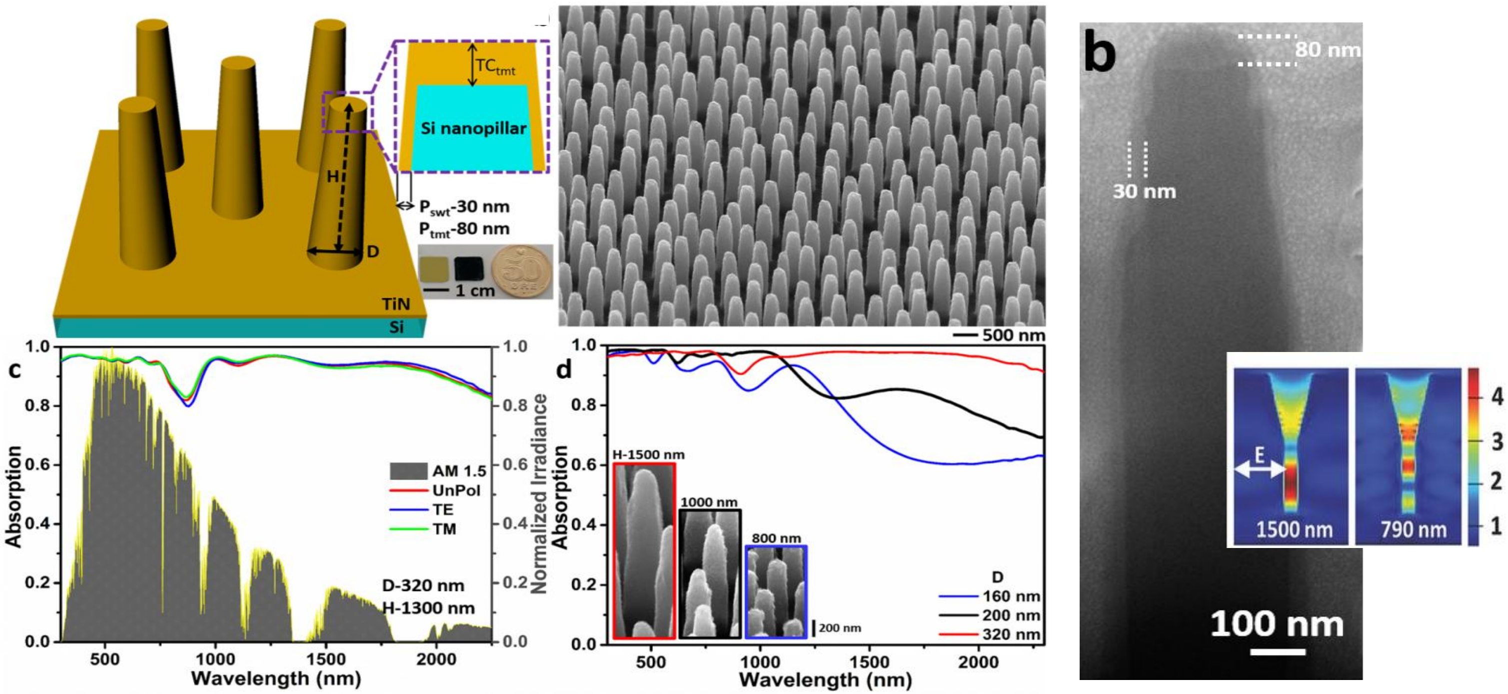
Higher losses – limits plasmon propagation

Optical Materials Express **8**, 3717 (2018).

3D TiN nanopillars for broadband absorption

TiN coated Si pillars

'Large area' - 1cm^2 - colloidal lithography

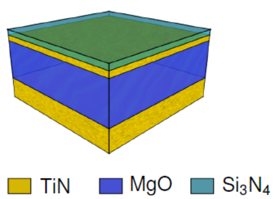


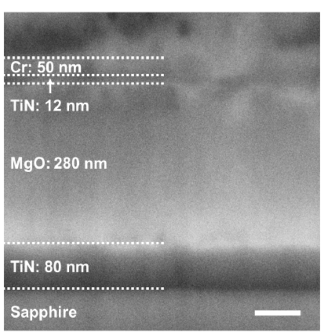
Vertical gap plasmon modes
Spectra tuned by height and density of pillars

Advanced Optical Materials **5**, 1700552 (2017)

Titanium nitride-Magnesium oxide based thermal emitter

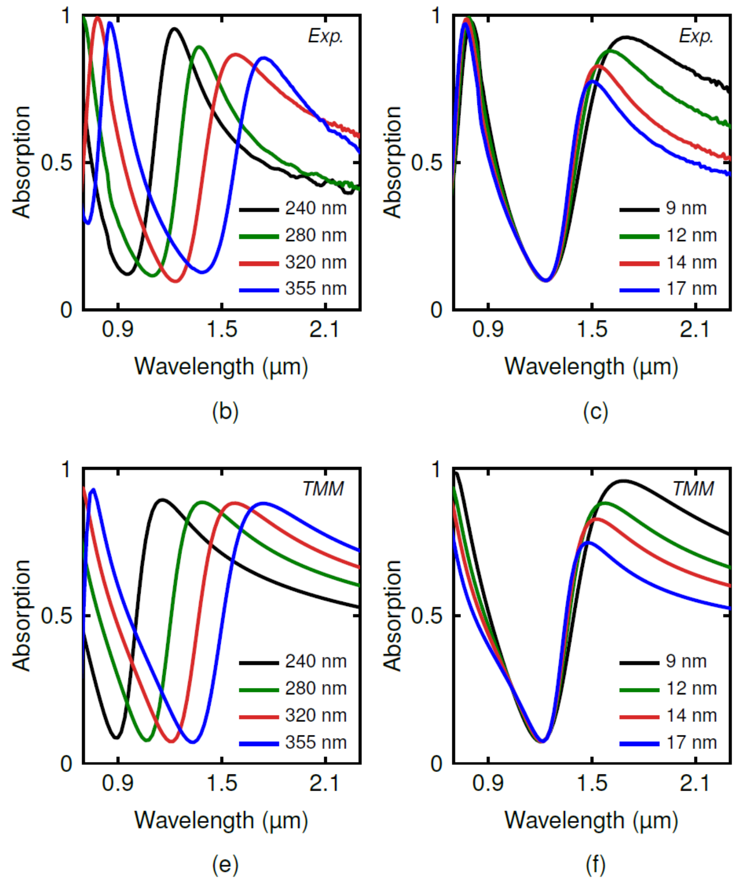
Metal-Insulator-Metal





Thickness MgO

Thickness top TiN



Optical Materials Express **8**, 3717 (2018).

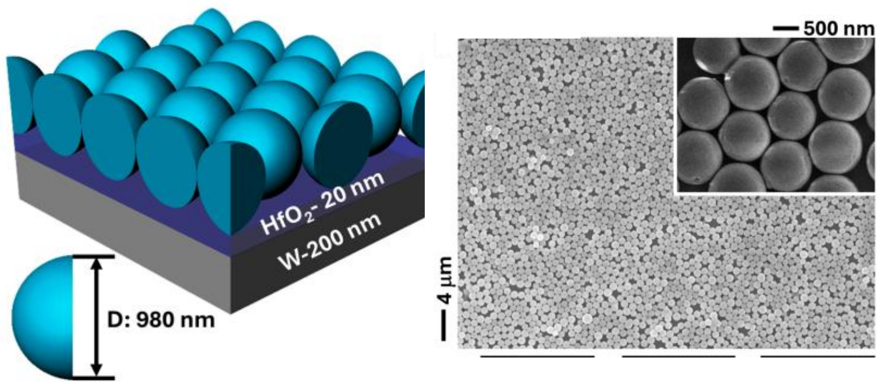
$$m \cdot 2\pi = \phi_{\text{prop.}} + \phi_{\text{r, bottom}} + \phi_{\text{r, top}}$$

New materials:
Melting point of Si is $1414^{o}C$
Protection layers (Si_3N_4)

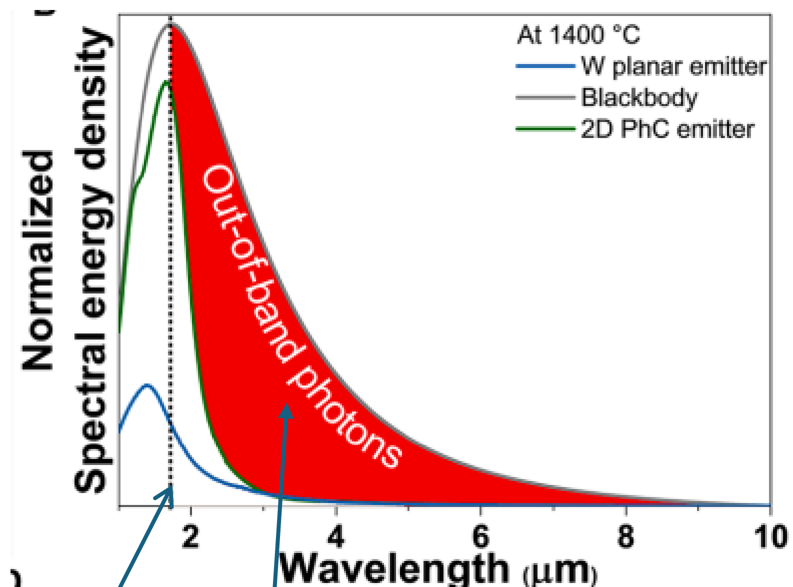
Design through geometrical parameters:
Thickness of dielectric
Thickness of top metal layer

Good agreement between experiment and theory

2D photonic crystal emitter



Simple and scalable self-assembly process



GaSb PV cell with 0.72 eV (1720 nm) band gap

Photons with energies above Eg do not contribute to PV current

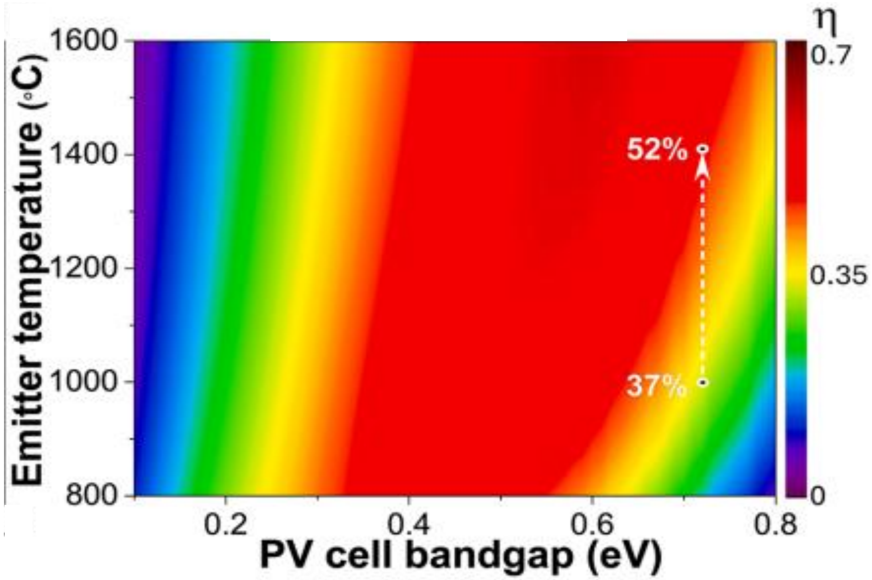
Design of spheres: Optics Express, 23, A1236-A1244 (2015)
https://doi.org/10.1364/OE.23.0A1236
Mie resonances, quadrupole from 1.56 µm, tunable with radius
Yttrium stabilize Zirconium, Stable to 1500 ºC

Cell Reports Physical Science (2025),
https://doi.org/10.1016/j.xcrp.2025.102850

Efficiency

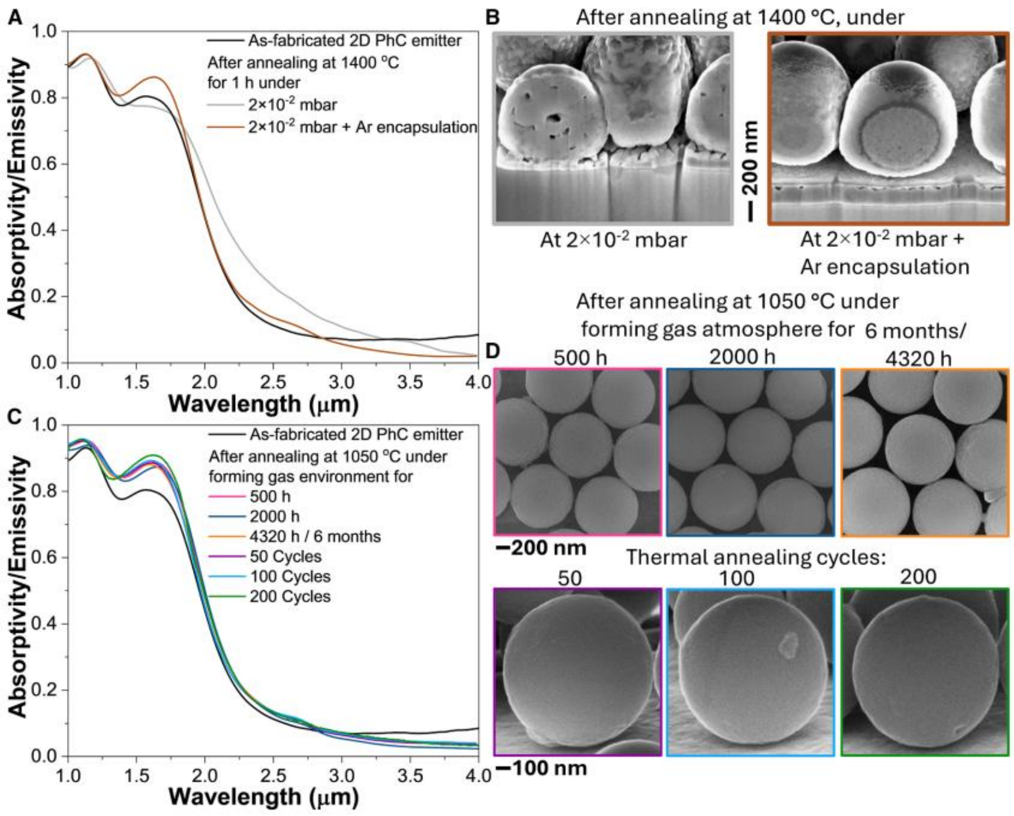
$$\eta = \int_{E_g}^{\infty} \frac{E_g}{E} \varepsilon(E) I_{BB}(E,T) dE \Big/ \int_{0}^{\infty} \varepsilon(E) I_{BB}(E,T) dE$$

η defines the ratio of the convertible thermal radiation energy by the PV cell to the total radiated thermal energy by the emitter



Optical efficiency 52 % at 1400 °C

Thermal stability



Stable at 1400 ℃ for an hour
With Ar protection

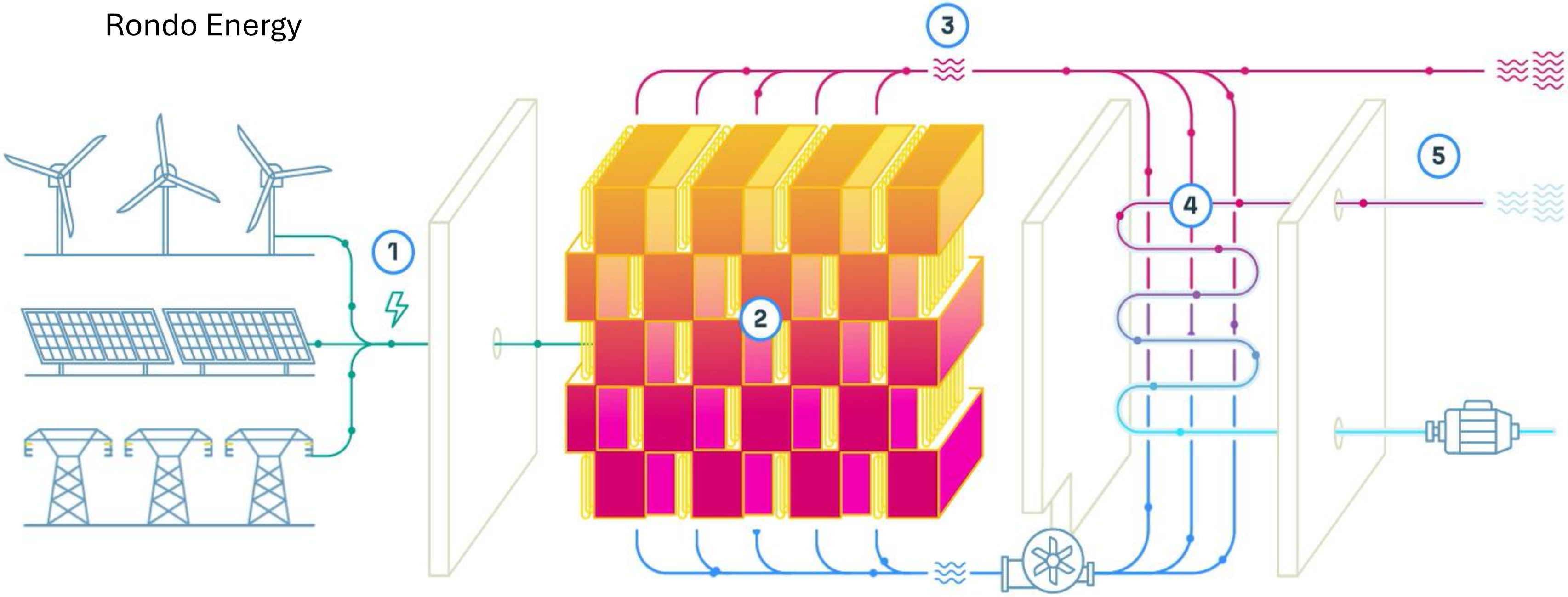
Stable at 1050 ℃ for half a year
in forming gas atmosphere (N2/H2)

Potentials in TPV

- Solar - CSP systems, eg. tower concentrators
- Waste energy
  - Industrial production
- Thermal batteries (next slides)
- Energy source at remote places
  - Solar
  - Nuclear
  - . . . .

Storage: The usual thermal solution- turbines

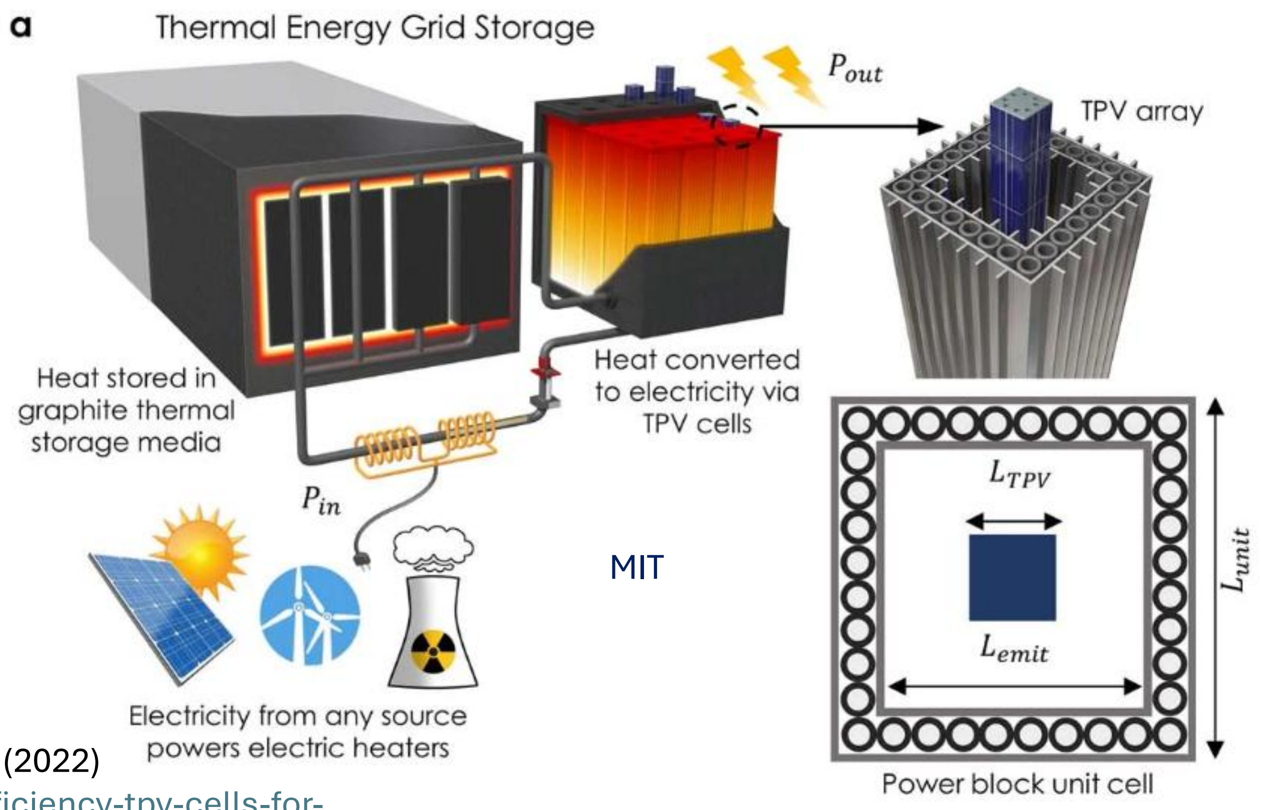
Rondo Energy



Thermal energy to electricity- TPV

Heat to electricity

Antora, California



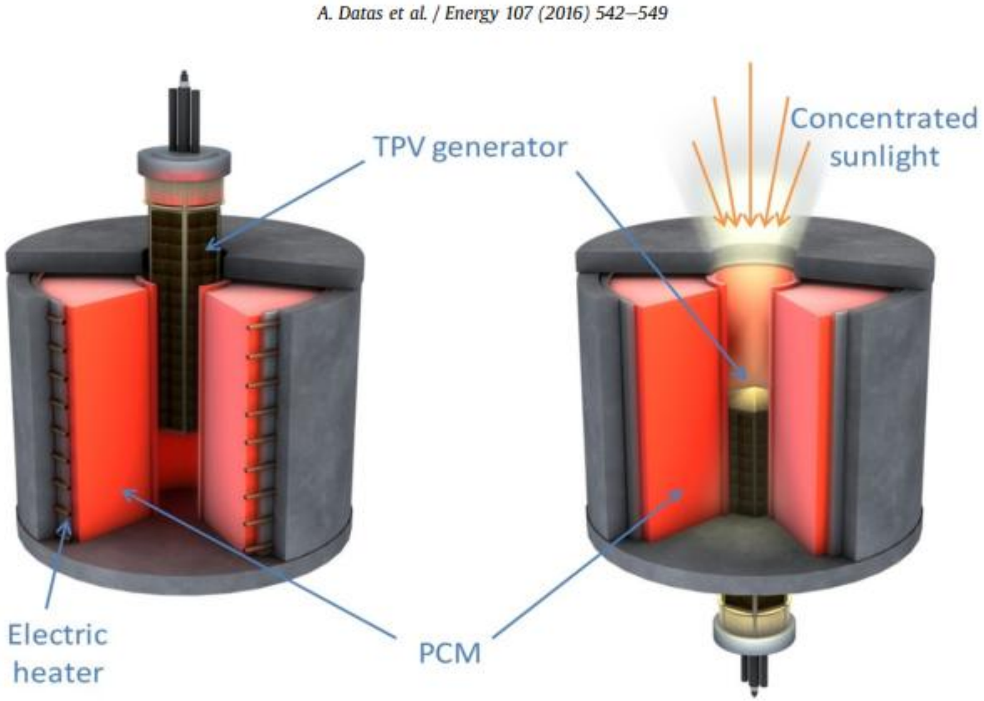
MIT

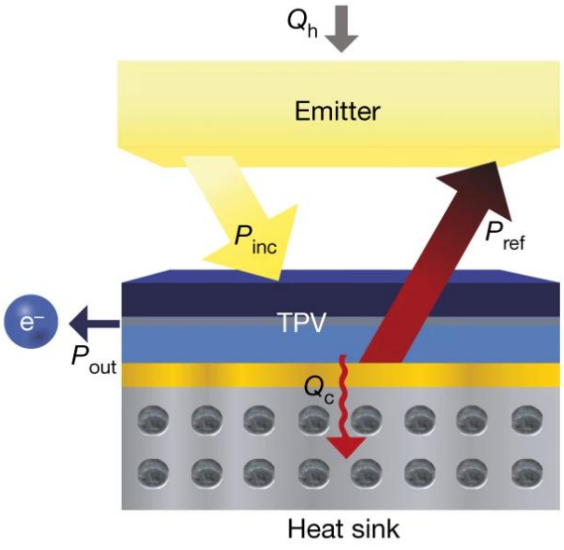
https://www.antora.com/company

Nature **volume 604**, pages287–291 (2022)

https://eepower.com/news/high-efficiency-tpv-cells-for-grid-scale-thermal-batteries/#

Thermal batteries – with TPV





Backside cooling
Reflector

Power–to–X

- Electricity from Solar and Wind to liquid fuels (e-fuels)
  - Hydrogen
  - Hydrogen + Carbon (CO_2) or Nitrogen -> Ammonia, Methanol, Methane, ..

CAPeX

Pioner Centre for Accelerating P2X Materials Discovery

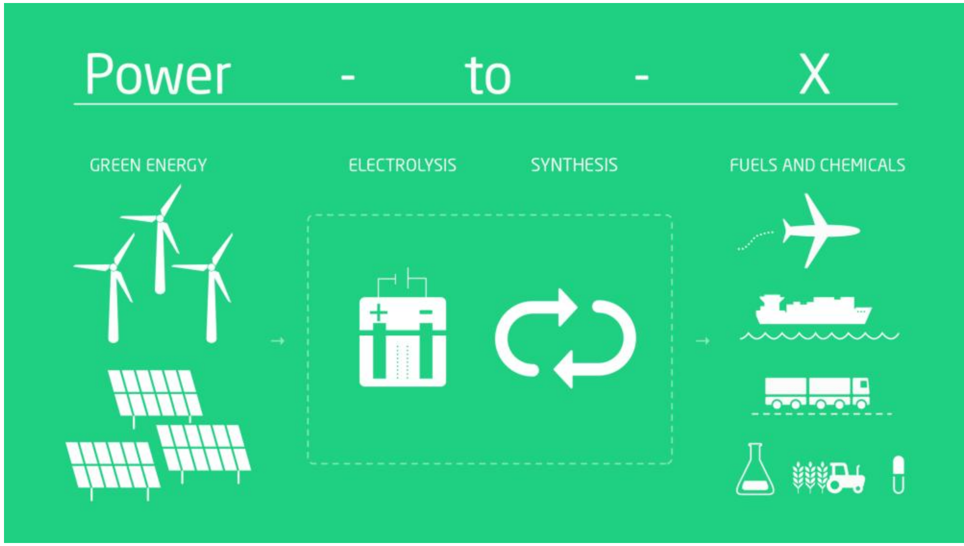
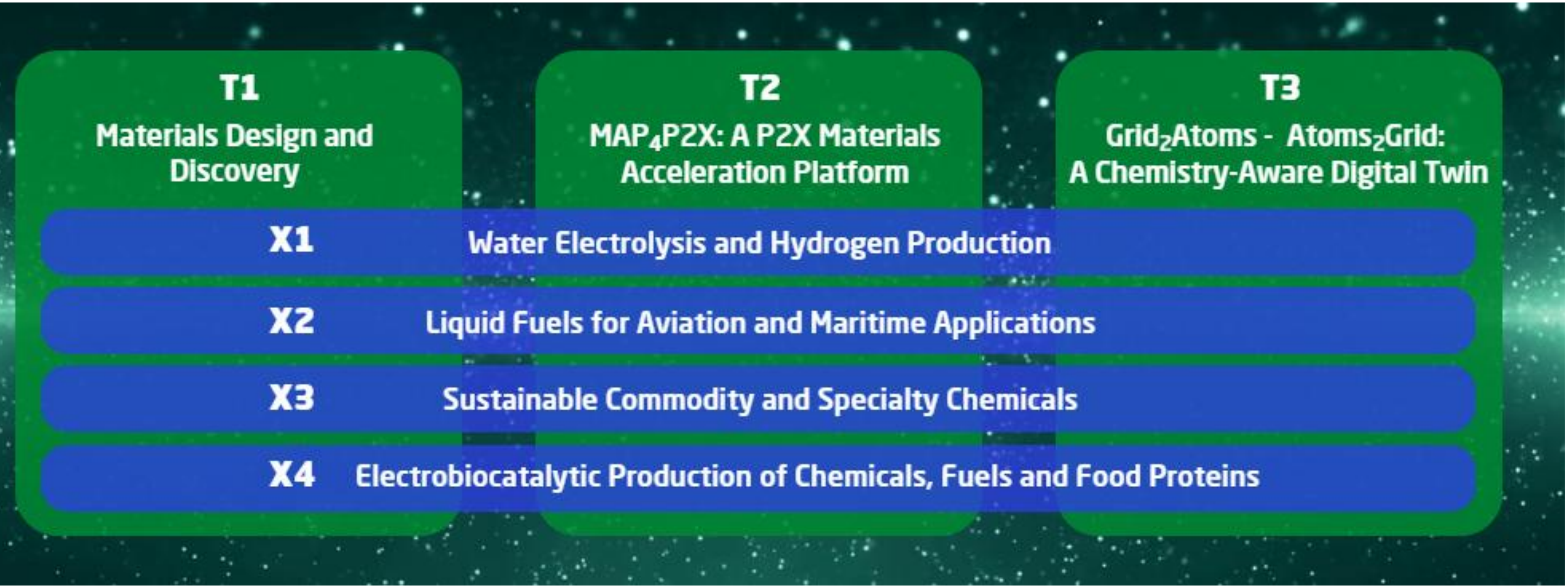


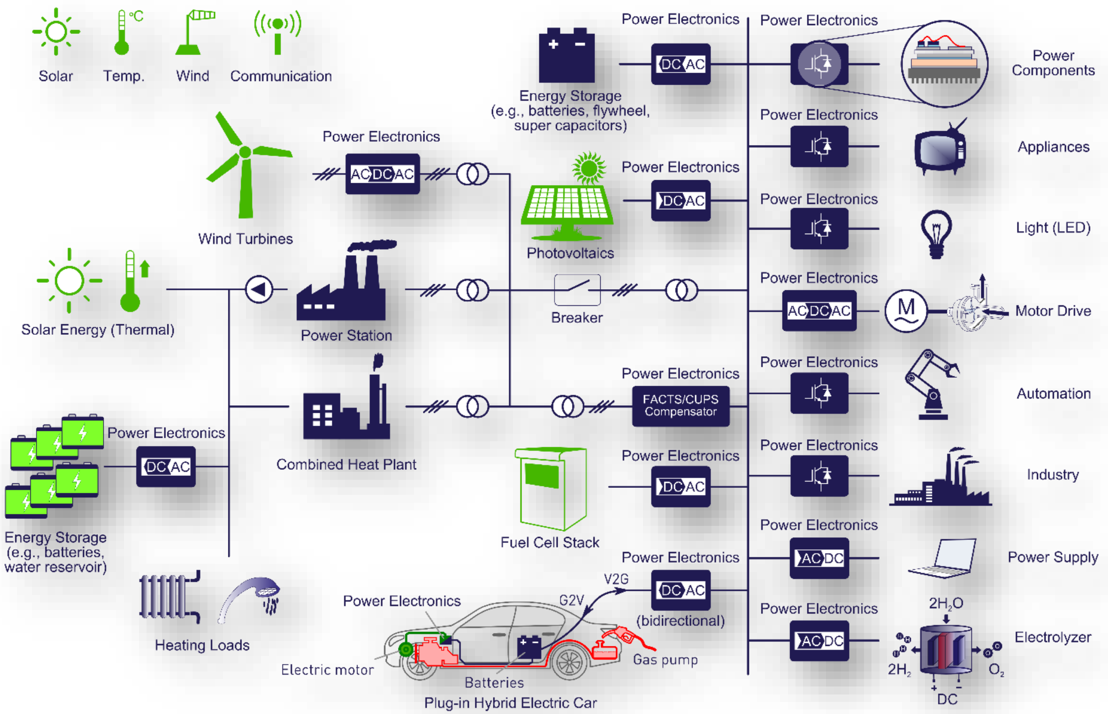
Illustration showing the individual parts of Power-to-X.
Illustration: DTU

CAPeX


T1
Materials Design and Discovery
T2
MAP4P2X: A P2X Materials Acceleration Platform
T3
Grid2Atoms - Atoms2Grid: A Chemistry-Aware Digital Twin
X1
Water Electrolysis and Hydrogen Production
X2
Liquid Fuels for Aviation and Maritime Applications
X3
Sustainable Commodity and Specialty Chemicals
X4
Electrobiocatalytic Production of Chemicals, Fuels and Food Proteins

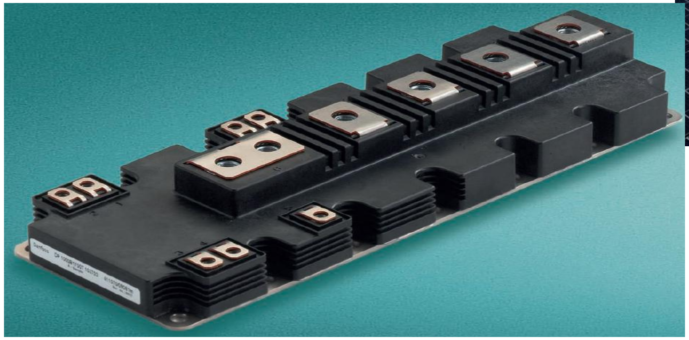
The electrical energy system

Power Electronics: Energy Production – Energy Distribution – Energy Consumption – Energy Control



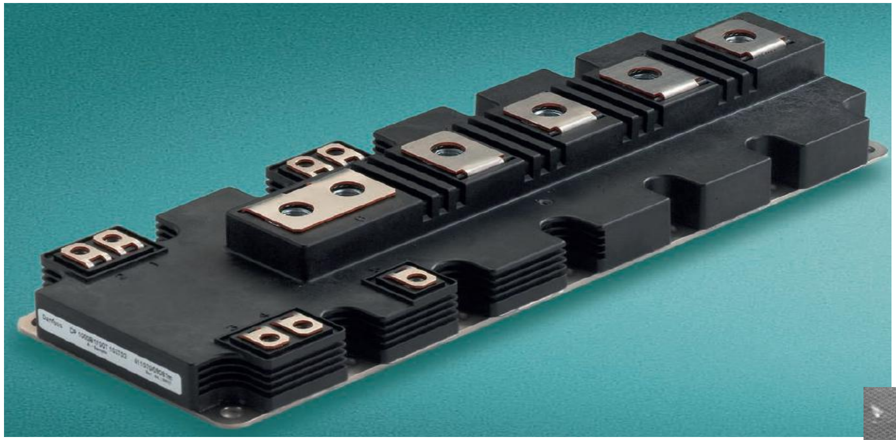
Power electronics

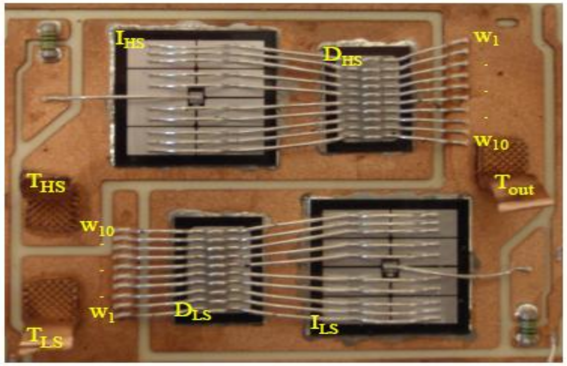
- 70 % of electricity is processed by Power Electronics
- This will increase in the future
- PE: the use of semiconductors to control and convert electrical power
  - Generation
  - Conversion
  - Consumption
- Reliability is essential



Materials science in power electronics packaging

Center for Reliable Power Electronics (CORPE)

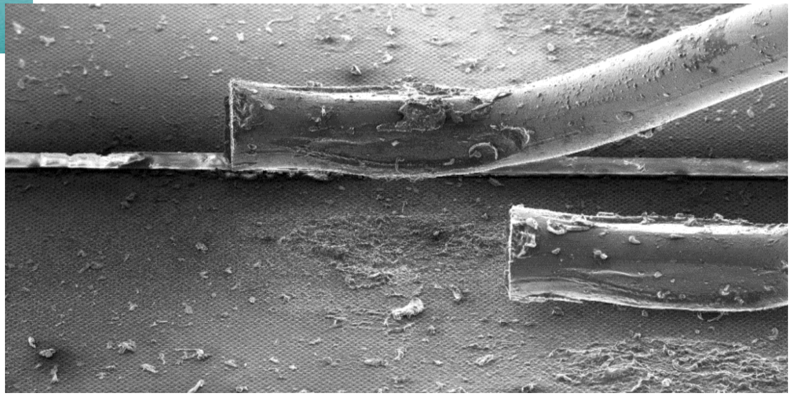




IGBT-module (Insulated Gate Bipolar Transistor)

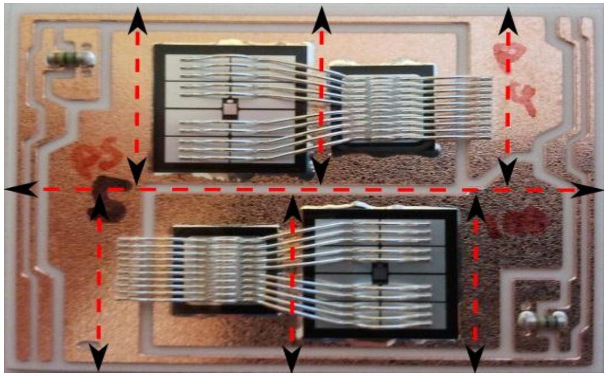
Modules wear out over time – finite lifetime

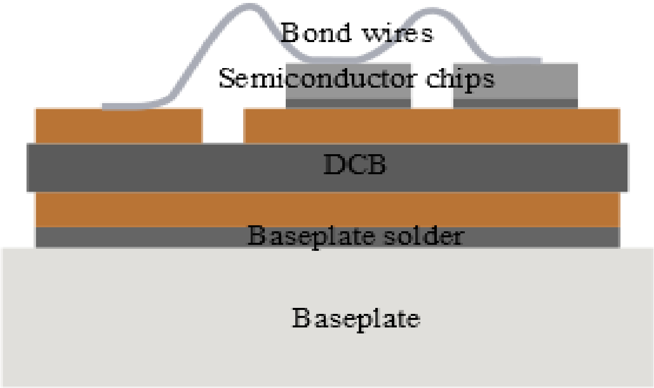
Thermo-mechanical stress cycles



Micro-Sectioning

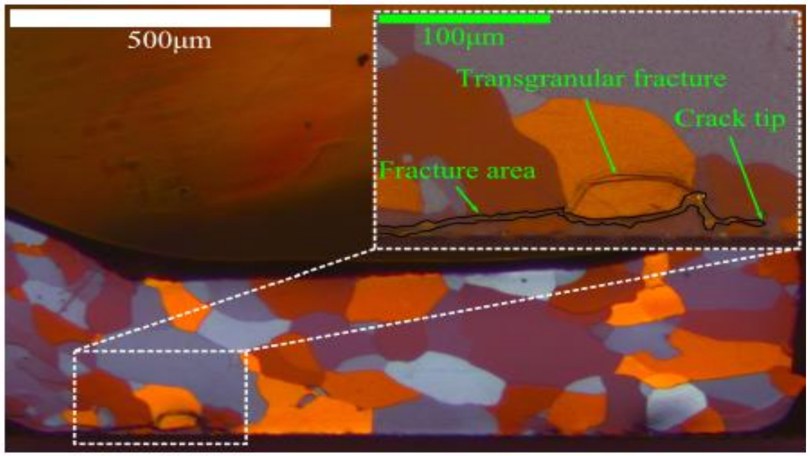
- Separation of section
  - 2xIGBT and 2xDiode
- Embedding in epoxy and removal of DCB and chip solder
- Embedding in epoxy for wire interface
- Electrochemical etching (2min, 30V, 1% Hydrofluoric acid)
- Microscopy

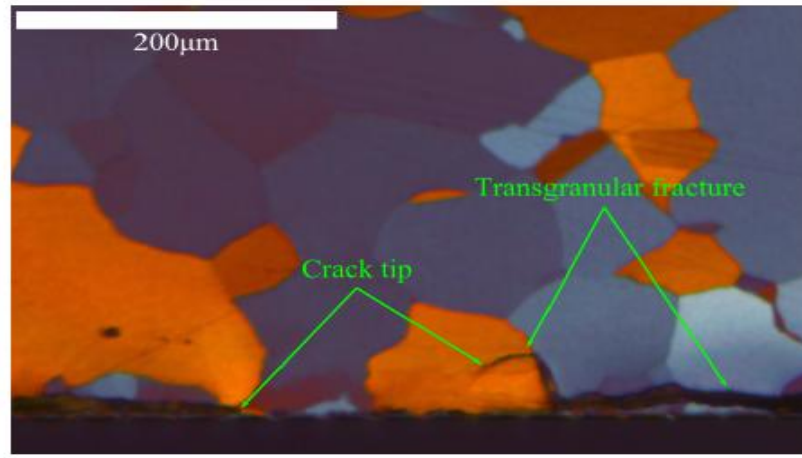




Microelectronics Reliability, Vol. 53, 1422-1426 (2013)

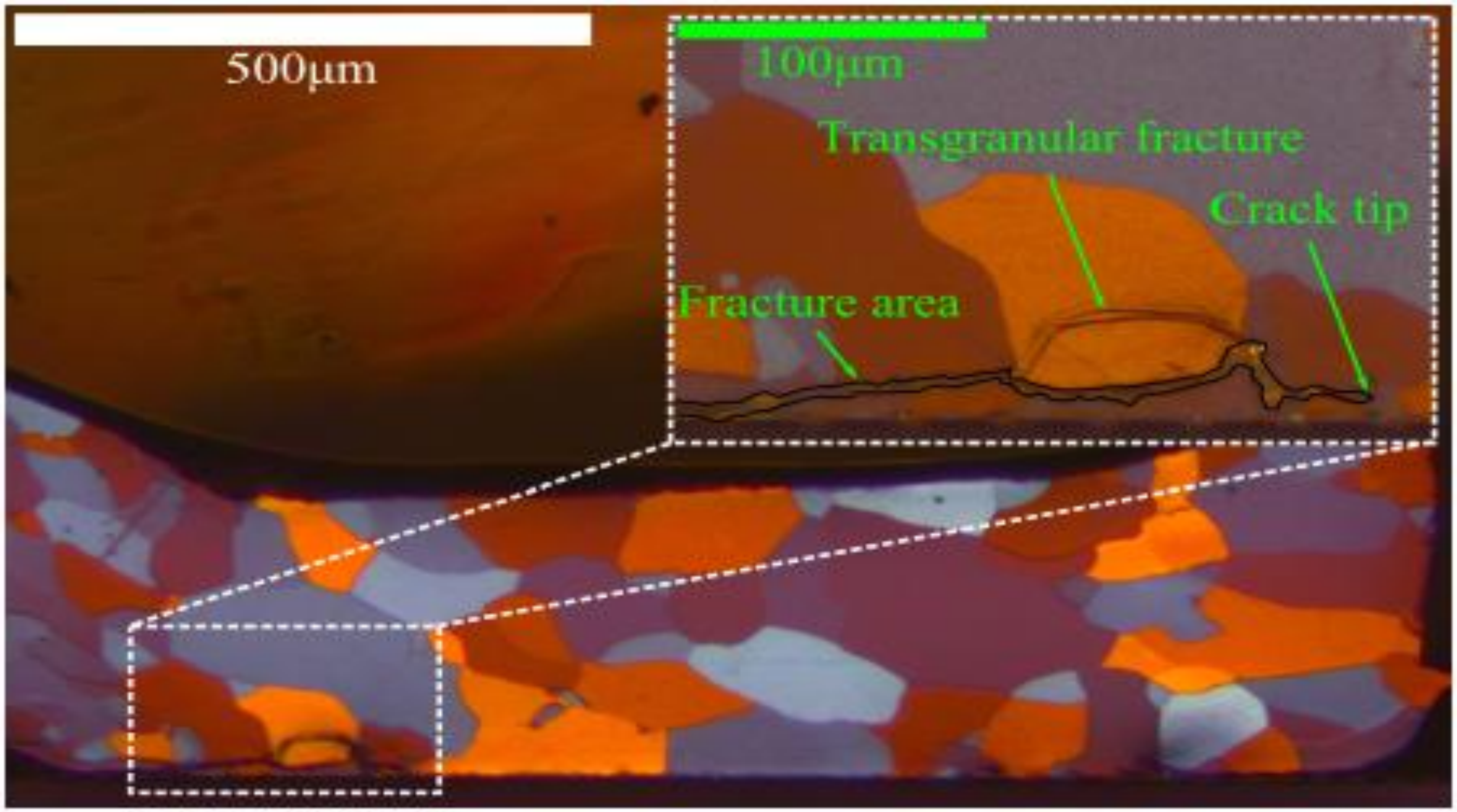
Bond wire fatigue





Cracks develop near interface between bond wires and metallization layer.
Follows grain interfaces, but fractures through grains are also seen.
Grain sizes and gradients in sizes important parameters.
Follows large gradients in grain size.

Microelectronics Reliability, **58**, 58 (2016)


500μm
100μm
Transgranular fracture
Crack tip
Fracture area

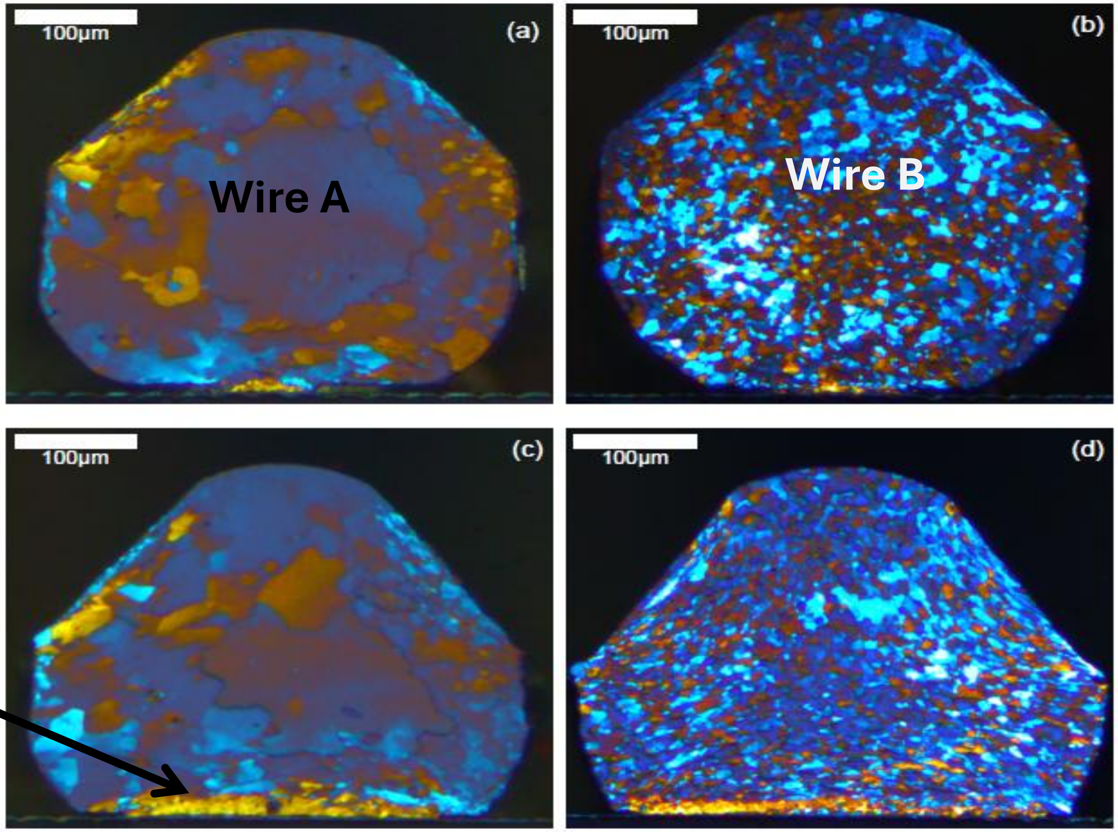
Wire cross sections

Cross sections inside and outside the bonding areas for two different types of wires.

Outside bonding

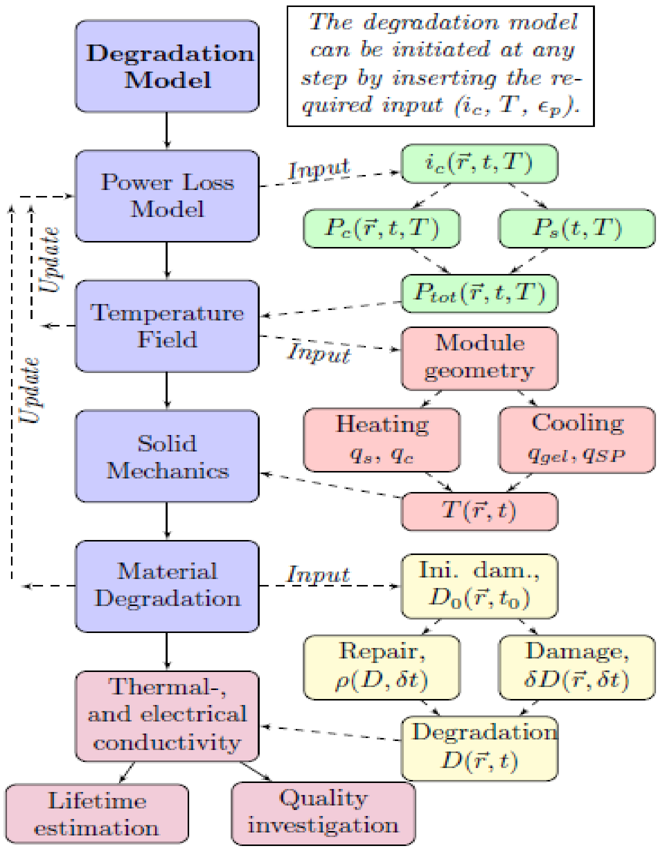
Inside bonding

Recrystallization area



Journal of Materials Science: Materials in Electronics, **25**, 2863 (2014)

Modelling of thermo-mechanical failures



Thermal sources in the system

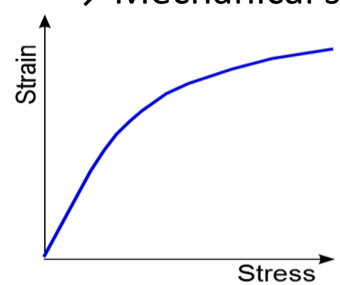
$$P_c^{IGBT} = i_c(\vec{r},t)v_{CE}(\vec{r},t,T)\left(\frac{1-m}{2}\right),$$

$$P_s^{IGBT} = f_s\left[E_{on}(T)+E_{off}(T)\right]\left(\frac{V_{DC}}{V_{ref}}\right)^{K_v^I},$$

$$P_c^{Diode} = i_F(\vec{r},t)v_D(\vec{r},t,T)\left(\frac{1+m}{2}\right),$$

$$P_{rec}^{Diode} = f_s\left[E_{rec}(T)\right]\left(\frac{V_{DC}}{V_{ref}}\right)^{K_v^D},$$

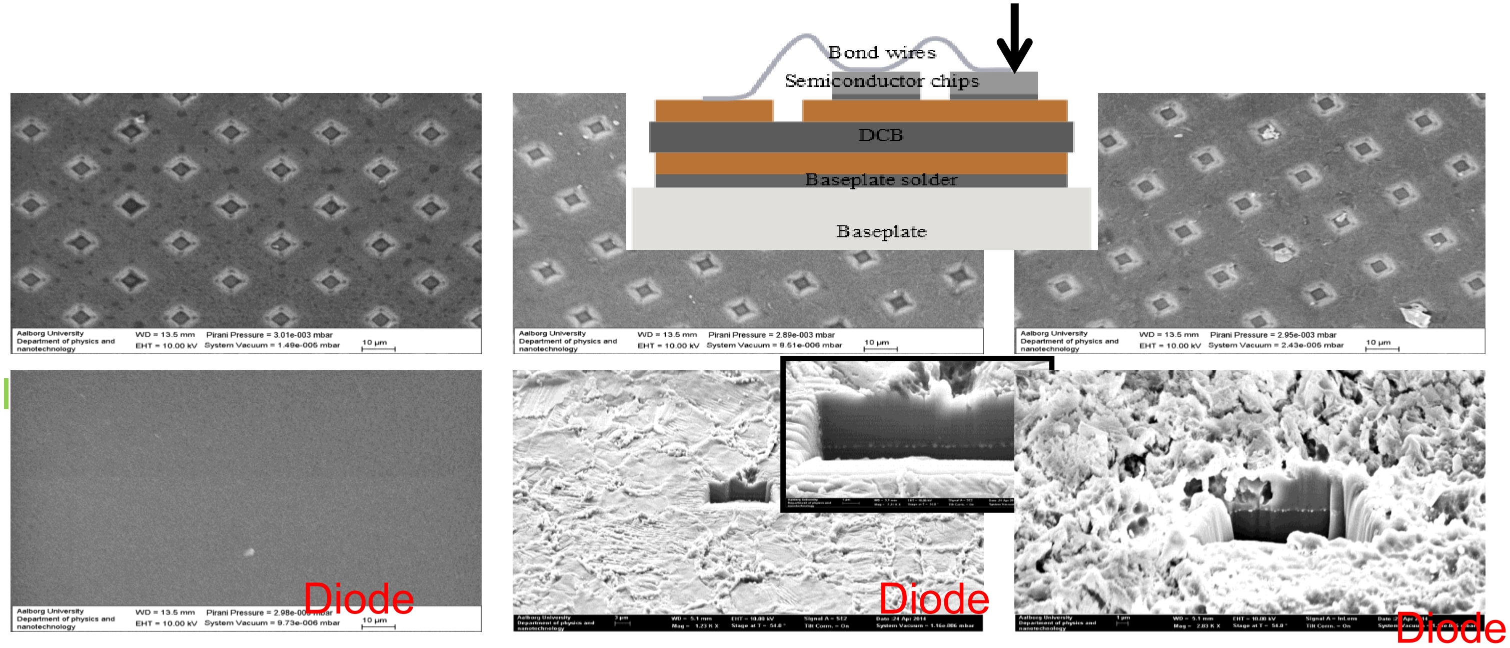
Differences in thermal expansion
→ Mechanical stress



Deformations beyond the linear range
→ Energy deposited in Structure for each cycle
→ Cracks

IEEE Trans. Power Electronics, **31**, 975 (2015)

Metallization Reconstruction



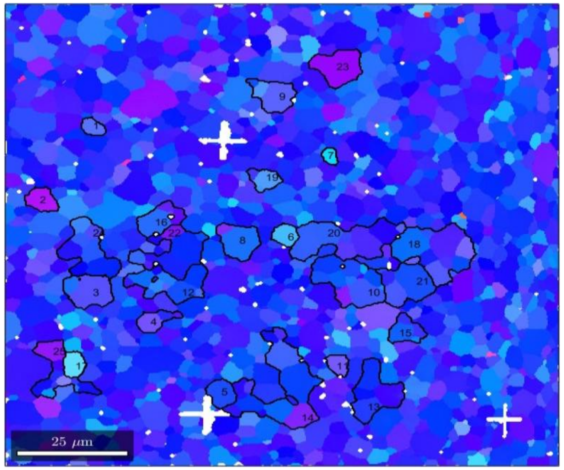
Thermal cycling leads to reconstruction of metallization layers

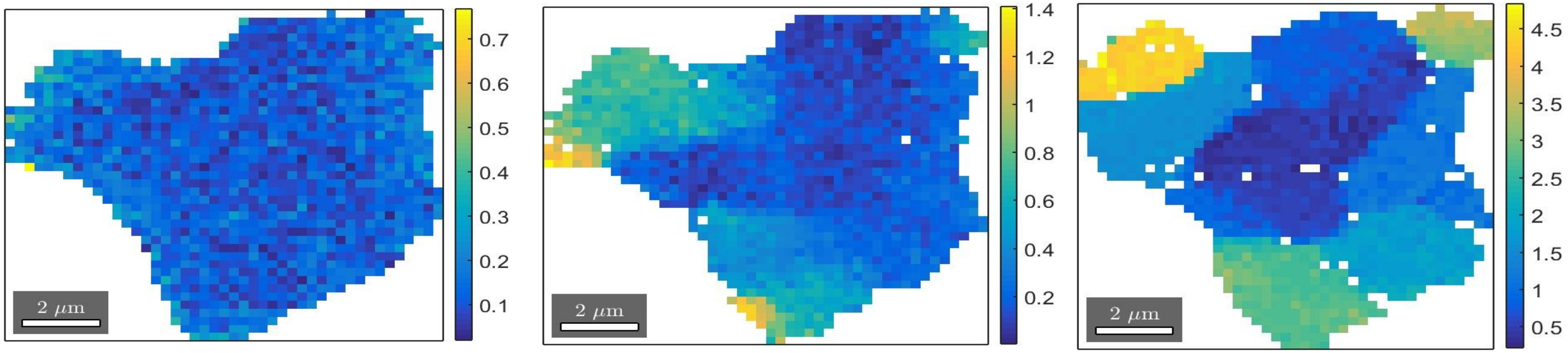
Electron Back Scatter Diffraction

- Detect diffraction pattern of electron beam to determine crystalline structures
- Create maps to determine grain size distribution and preferred grain orientation
- Track individual grains through an experiment

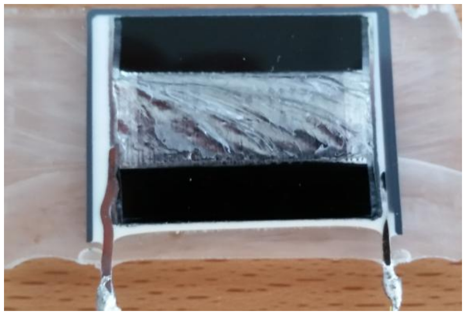
Seems to be purely thermal driven process
(no electromigration)

Journal of Materials Science: Materials in Electronics, 29, 3898 (2018)

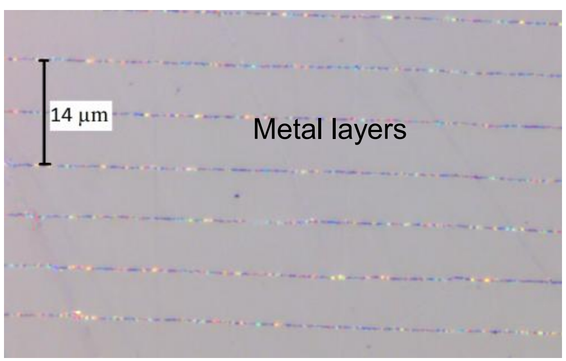




Thin Film Capacitors

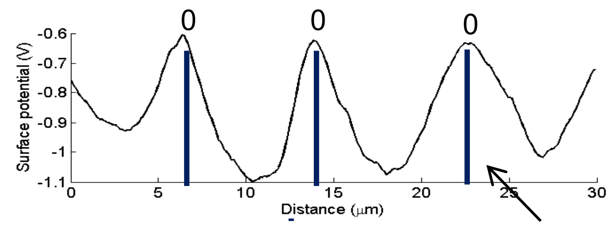


Section of TFC with wire connections

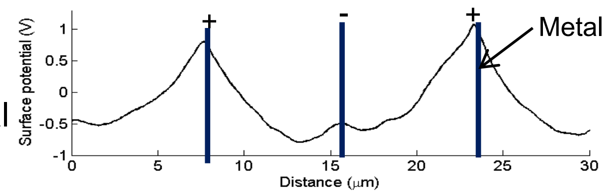


Kelvin Probe Force Microscopy

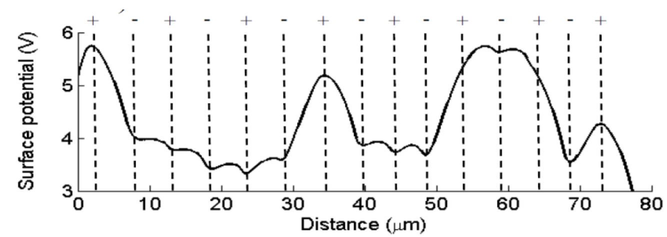
Reference Capacitor



5 V between adjacent metal layers



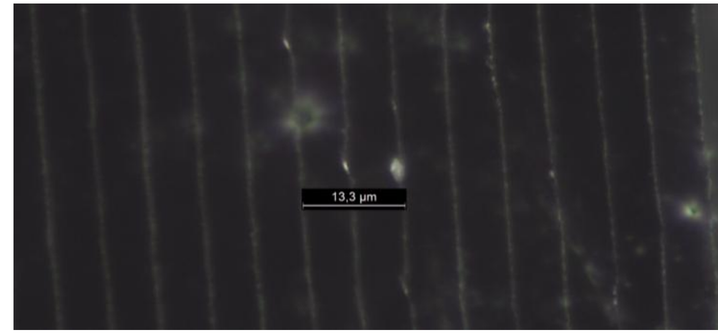
230 V, 85ºC
85 % HR
541 h



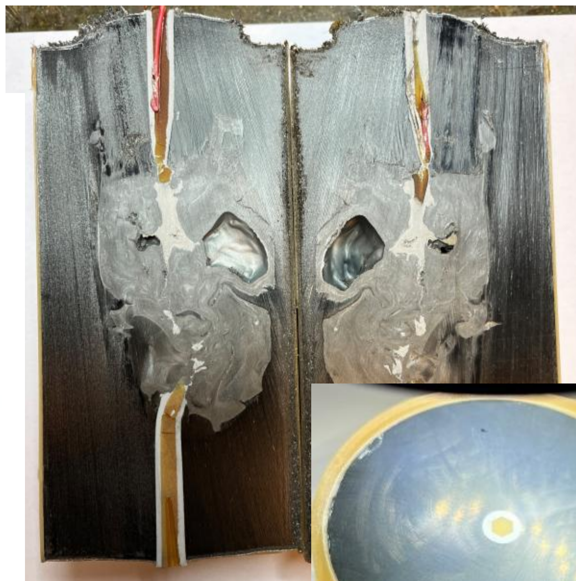
The stressed capacitor shows a poor connection through the metallization layers due to corrosion

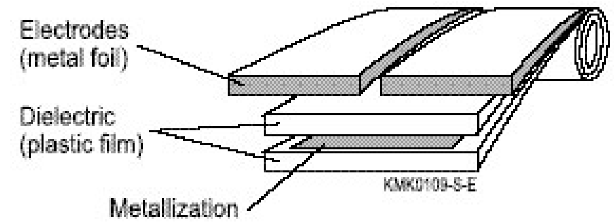
Annual Reliability and Maintainability symposium, 2015 proceedings

Power Capacitors



VISHAY power capacitors
3 cylindrical film capacitors





Polypropylene / Aluminum

Catastrophic breakdown

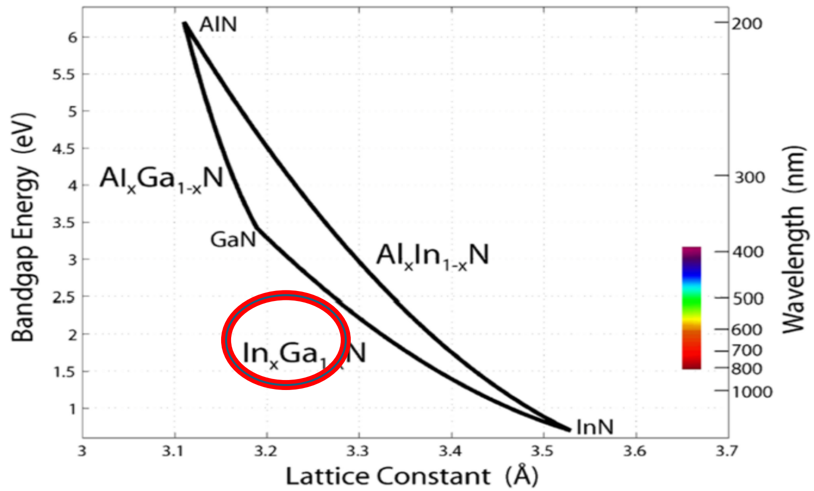
No electrical warning

No change in capacity up to breakdown

Semiconductors -devices

- Wide Bandgap Materials
  - GaN device layers
  - SiC device layers
- Future plans: Ultra Wide Bandgap semiconductors (Ga_2O_3, diamond..)

Nitride materials: Wide bandgap electronics

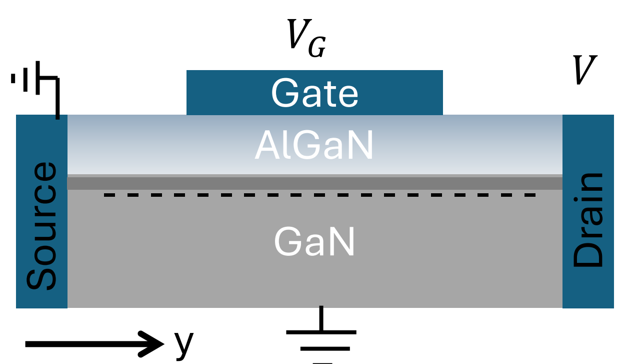


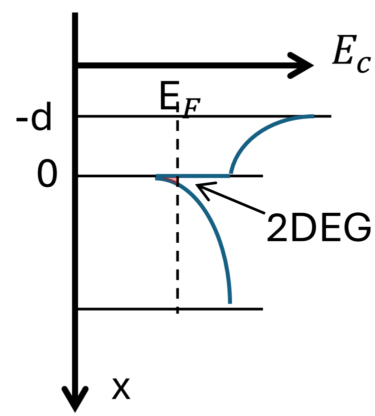
GaN diodes: Basis for white LED's
Nobel prize 2014

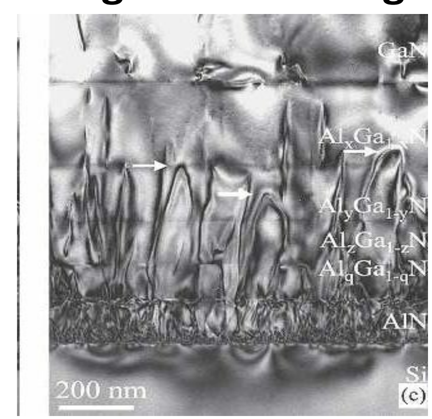
GaN basic properties:

- Band gap: 3.4 eV
- Thermal conductivity; 1.3 W/cm K (Si: 1.5)
- Hexagonal wurtzite structure
- Piezoelectric

Growth on Si wafers:
Main challenge is defect engineering

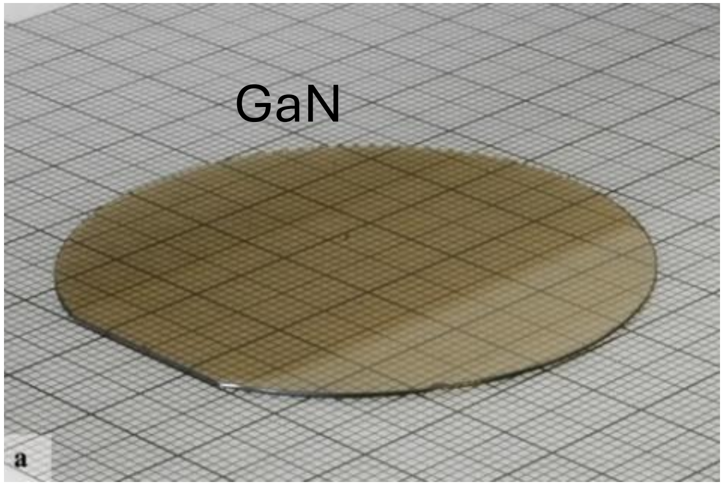






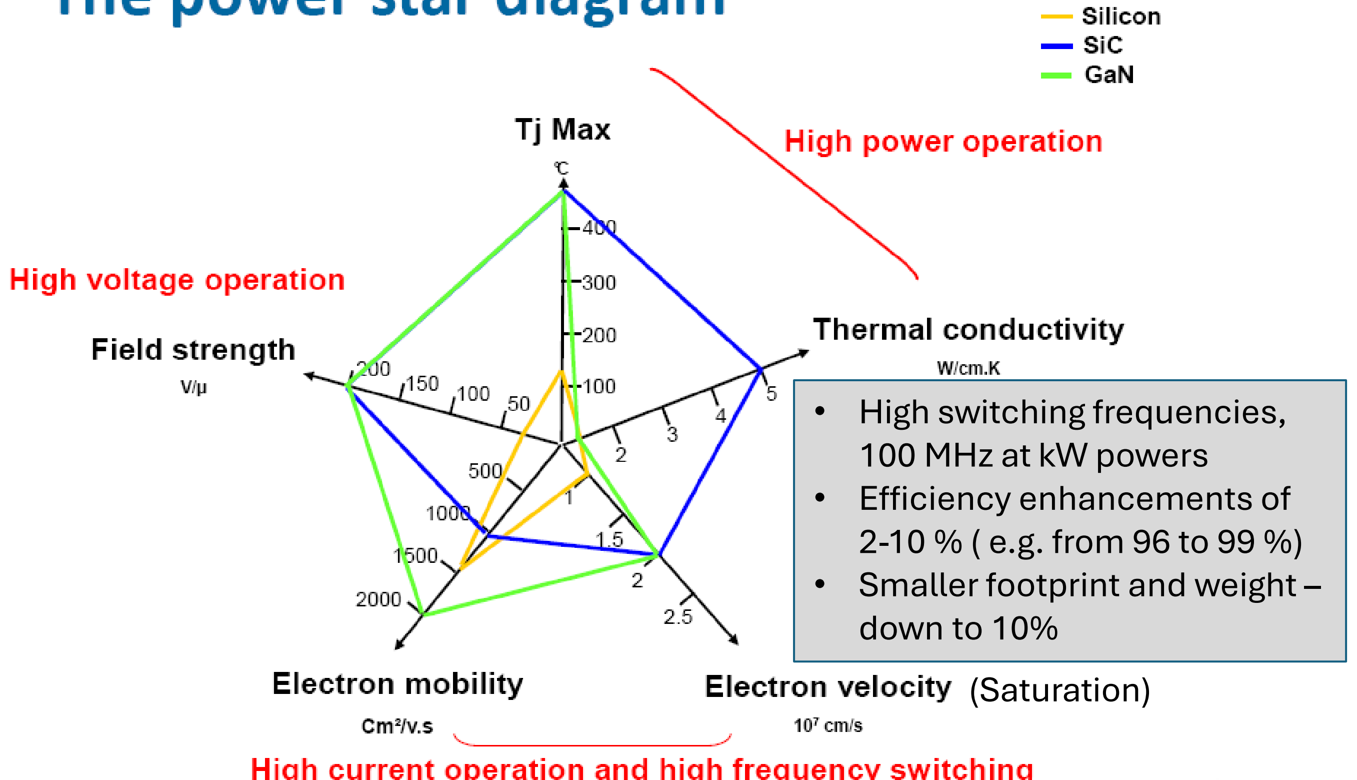
GaN – basic properties

- Must be grown as a thin film – large crystals not available like for Silicon
- Substrates: Sapphire (Al_2O_3), Silicon carbide (SiC), GaAs, **Silicon**
- Transparent in the visible
- Piezoelectric → transducers



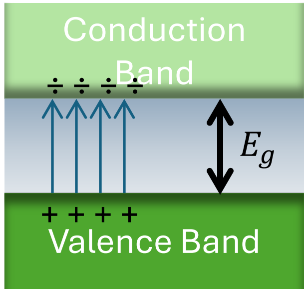
GaN and SiC potentials

The power star diagram



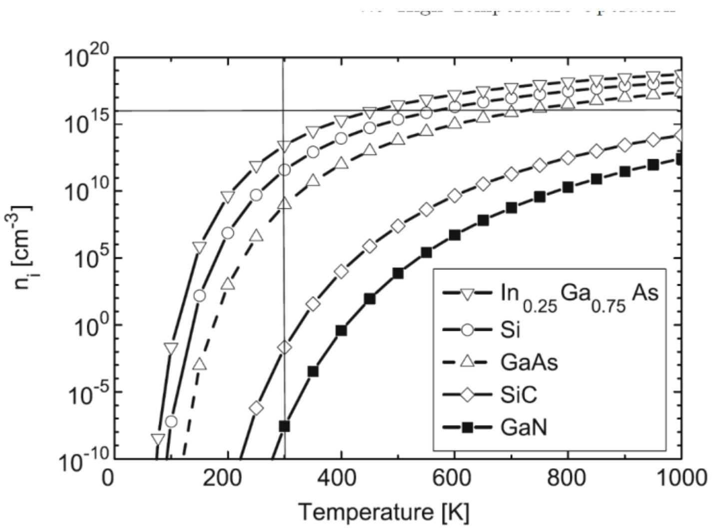
- High switching frequencies, 100 MHz at kW powers
- Efficiency enhancements of 2-10 % (e.g. from 96 to 99 %)
- Smaller footprint and weight – down to 10%

High Temperature Devices



Thermal excitation across the band gap:
All parts of semiconductor become conducting

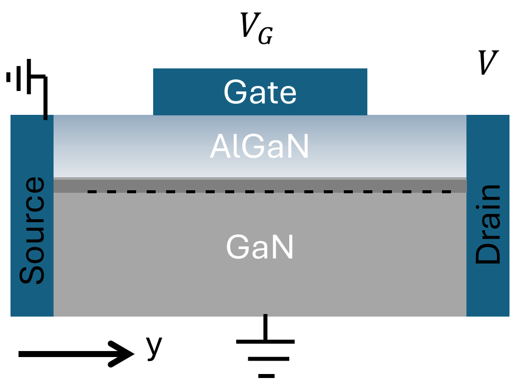
Advantage of wide band gap!

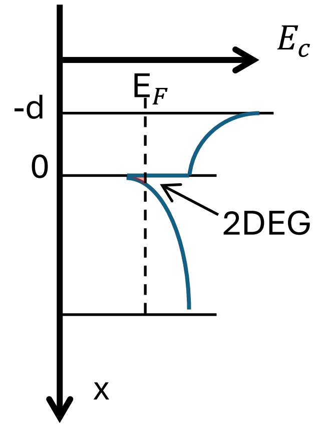


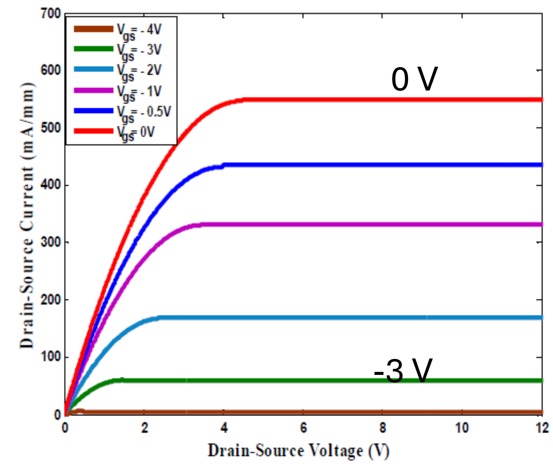
$$n_i = \sqrt{N_c N_v}\, exp\left(\frac{-E_g}{2k_B T}\right)$$

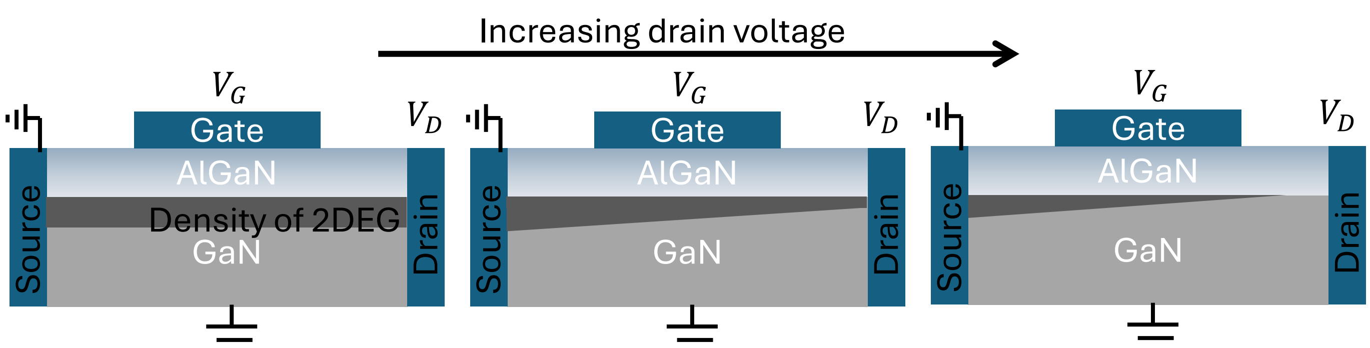
$$N_c, N_v\ density\ of\ states$$

IV characteristics









New materials are driving the green transition

- Efficiency of new technologies
  - New solar PV solutions
  - Catalysis: Power-to-X

- Lifetime of systems
  - High temperature materials
  - Corrosion
  - Thermomechanical design
- Circular materials
  - Design for reuse
  - Recovery of critical materials
- Critical raw materials
  - Replacements for scarce materials