Summer school on Epitaxy
MATEPI 2025
Porquerolles June 22-27 2025

Functional Metal-Oxides

from front-end materials research to platform for devices integration

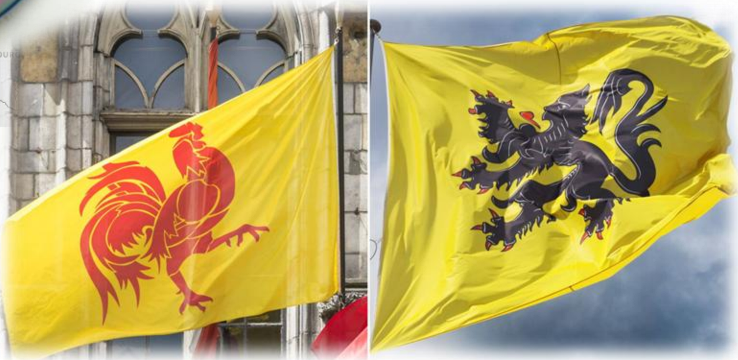
Prof. Dr. Clement MERCKLING
June 25st, 2025

Belgium

The country of …

Belgium

The country of …



Leuven, the Belgium Silicon Valley !

Arenberg Castle (Engineering faculty)

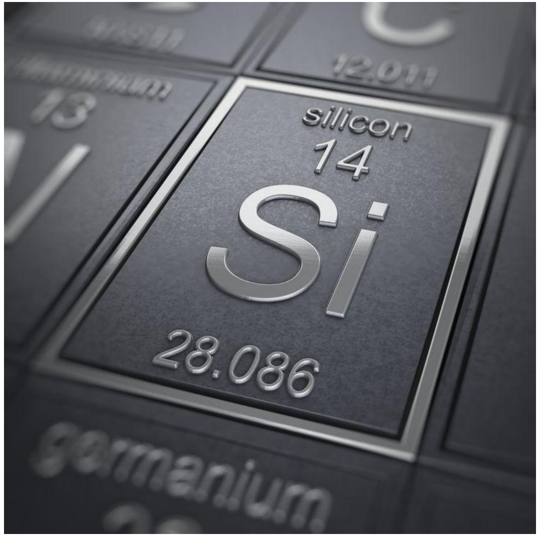
Materials Engineering Department

imec campus

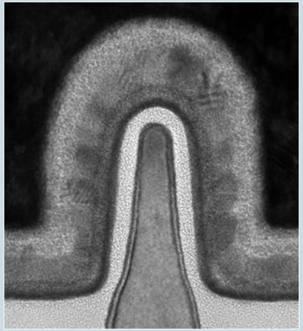
Imec in a nutshell

- imec
  - Started in 1984 (initial staff: 70 persons)
  - > 6 000 imec'ers
  - > 95 Nationalities
  - World-wide implantation
- Finances
  - > 1000 M€
  - > 75% industrial partners
- Main activity
  - R&D and innovation hub in nano-electronics and digital technology
- Core competences
  - Driving microchip miniaturization
  - Internet of everything
    - Smart health, food, automotive, city, technology, & energy

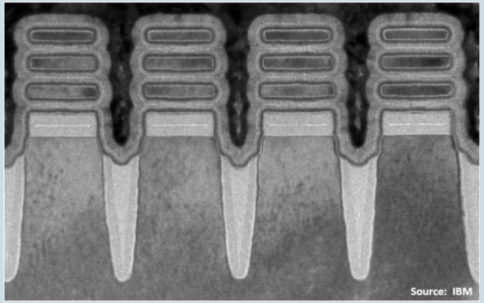
Unbeatable Silicon …



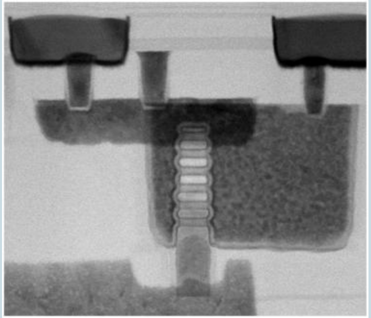
FinFET



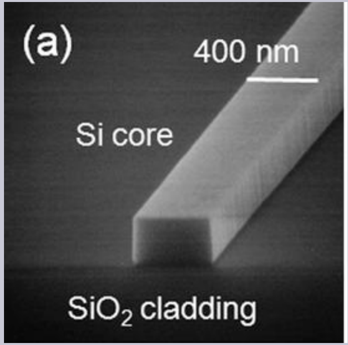
GAAFET


Source: IBM

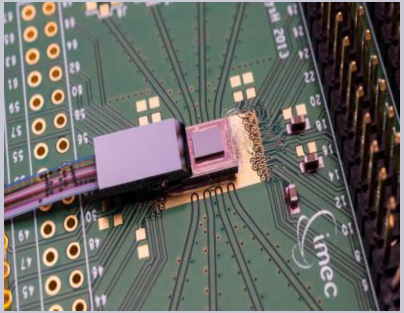
CFET



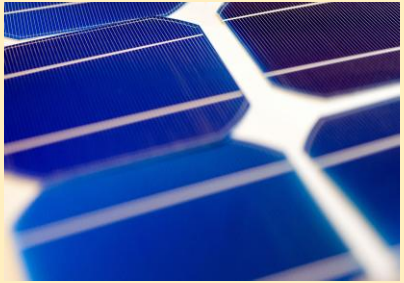
WGs



PIC

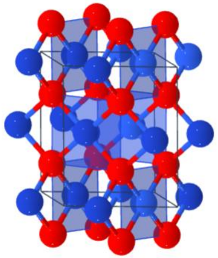


Solar

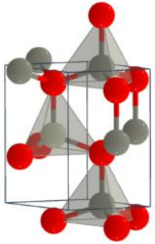


Zoo of oxides materials

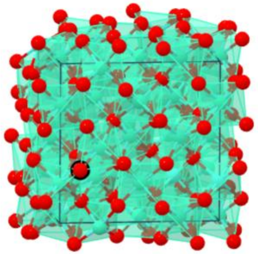
CuO



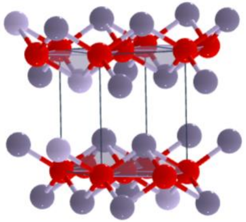
ZnO



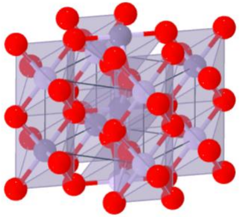
Gd_2O_3



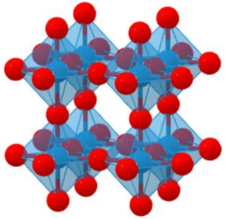
SnO



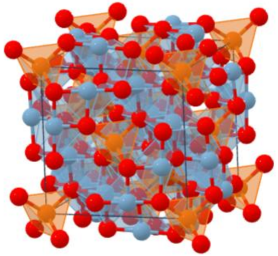
SnO_2



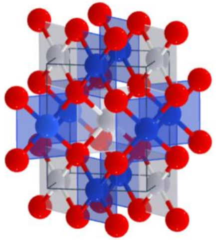
WO_3



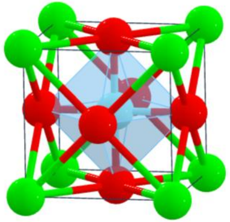
$MgAl_2O_4$



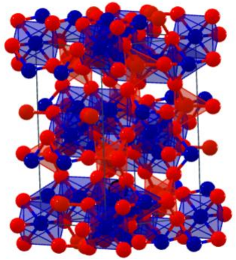
$PtCuO_2$



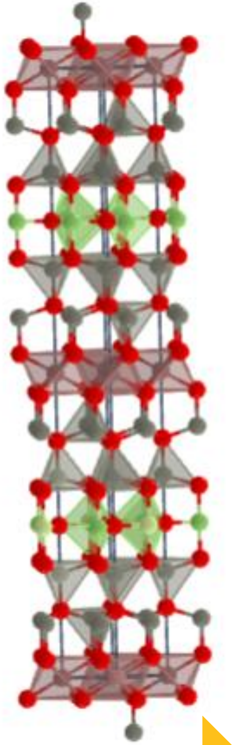
$SrTiO_3$



$Co_3V_2O_8$



$InGaZn_4O_7$

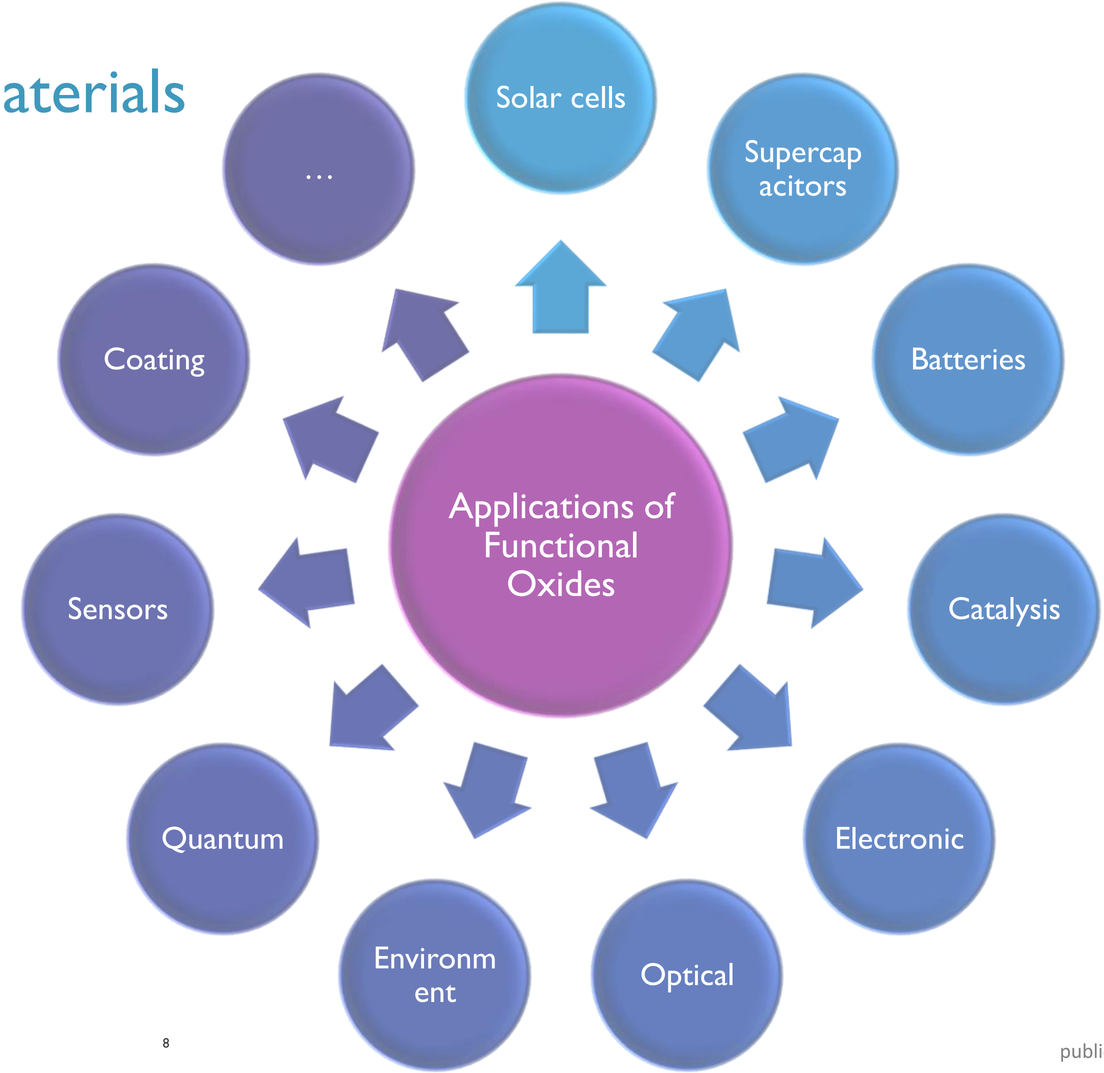


Binary

Ternary

Complex

Functional (Metal-)Oxides Materials



Applications of Functional Oxides

Solar cells

Supercapacitors

Batteries

Catalysis

Electronic

Optical

Environment

Quantum

Sensors

Coating

…

Functional Oxides Materials

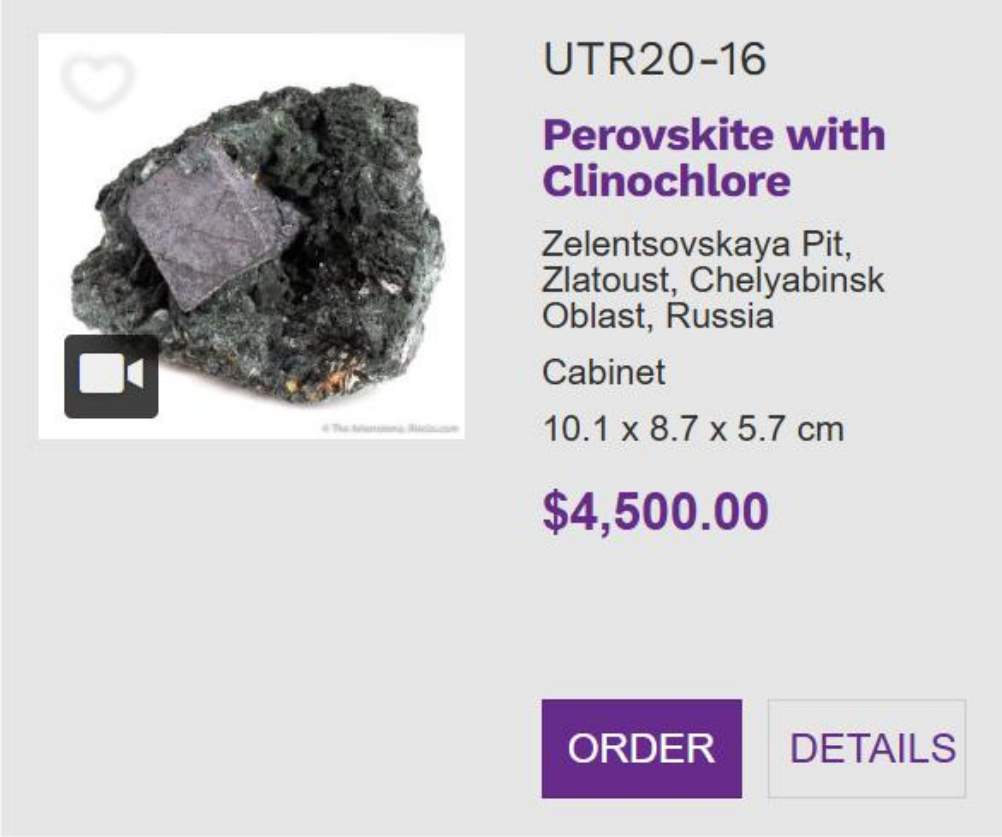
My favorite ?

Perovskite

- Discovered in 1839 by Gustave Rose while exploring the Ural mountains
- Calcium titanate ($CaTiO_3$) mineral
- Named in honour of Lev Perovski a Russian mineralogist

My favorite ?

Perovskite



UTR20-16

Perovskite with Clinochlore

Zelentsovskaya Pit, Zlatoust, Chelyabinsk Oblast, Russia

Cabinet

10.1 x 8.7 x 5.7 cm

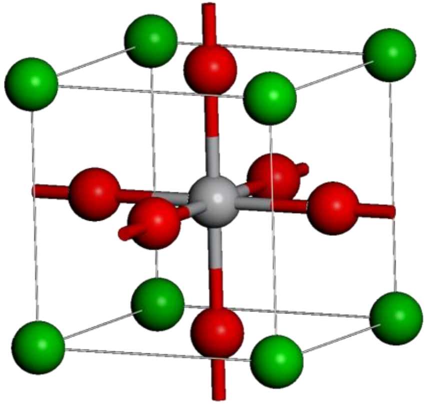
$4,500.00

ploring the Ural

ineralogist

Perovskite oxides

- Common structure & chemical formula ABO_3

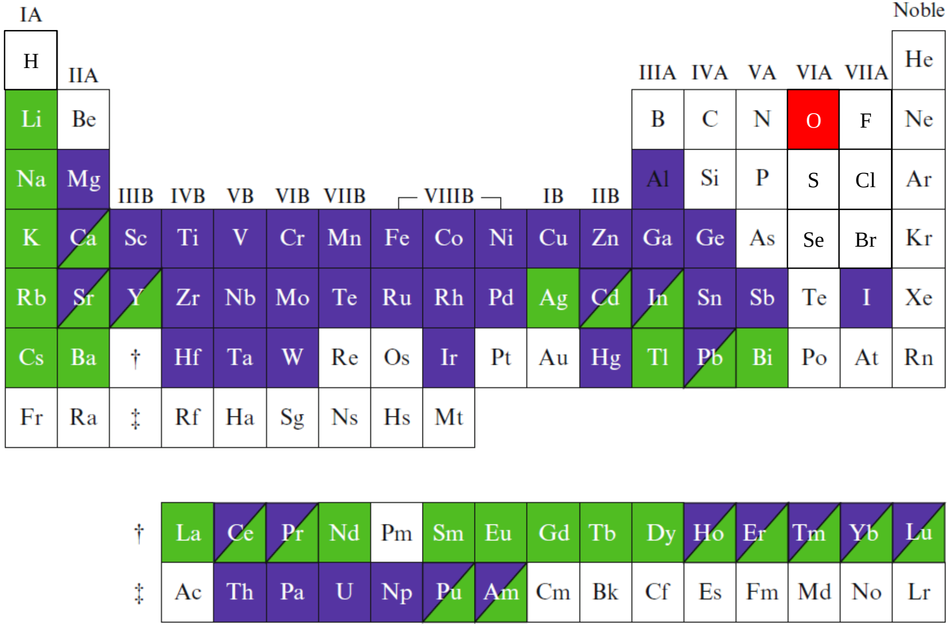


AO plane

BO_2 plane

Perovskite (ABO_3)

- Extensive number of combinations of elements
- Various properties…

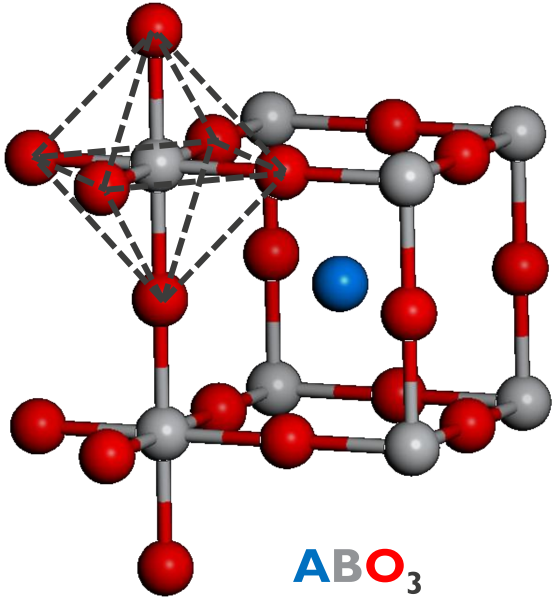


IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA	Noble
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Te	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	†	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	‡	Rf	Ha	Sg	Ns	Hs	Mt									
		†	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
		‡	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

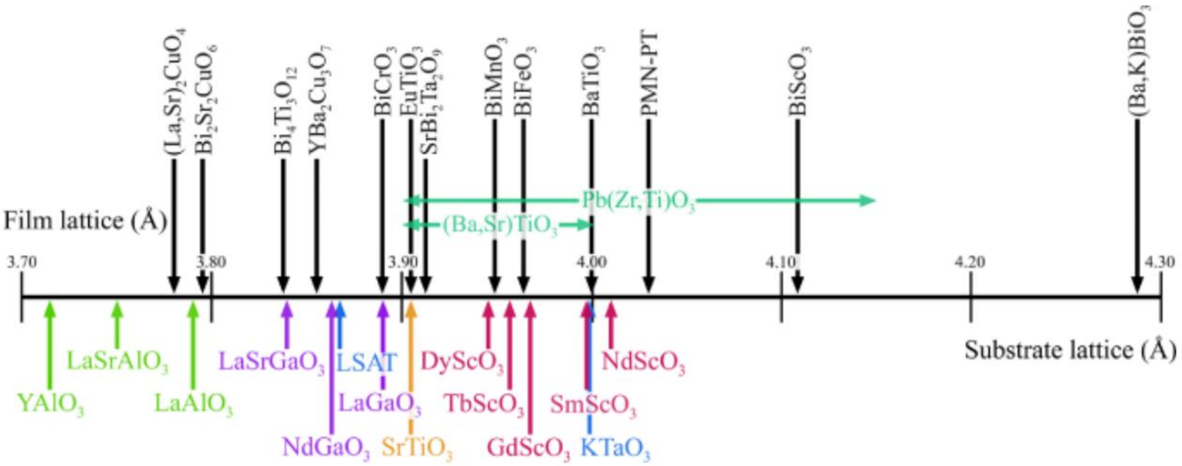
Perovskite oxides

Lattice parameter

$$a = 1.8836(r_B + r_O) + 1.4898\left[r_A + r_O\sqrt{2}(r_B + r_O)\right] - 1.2062$$



ABO$_3$

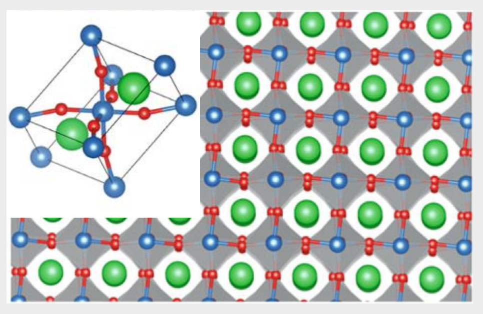


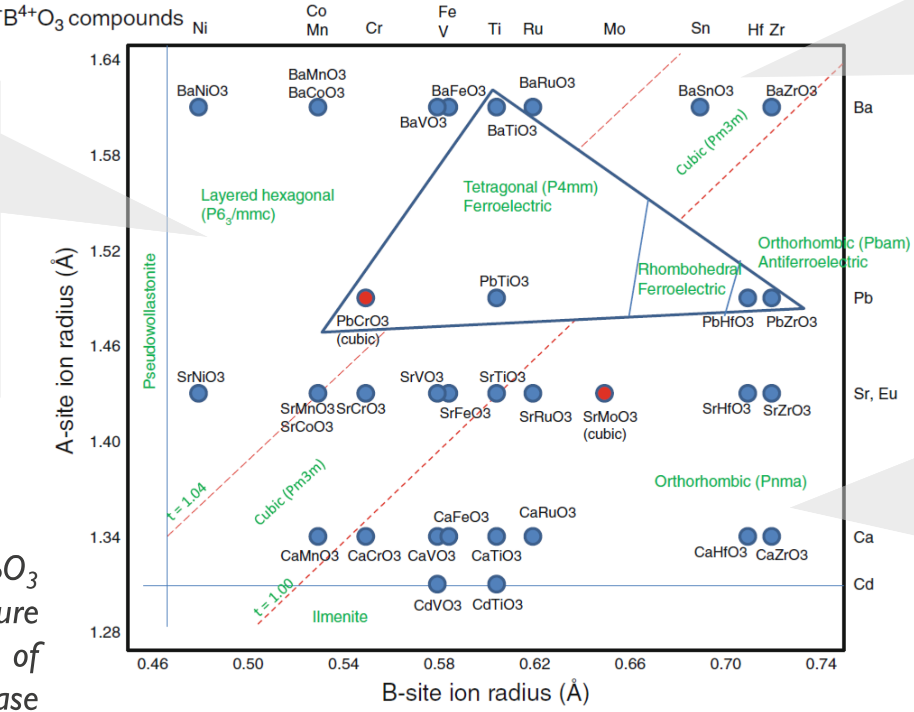
D. Schlom et al., J. Am. Ceram. Soc., 91; [8] 2429–2454 (2008)

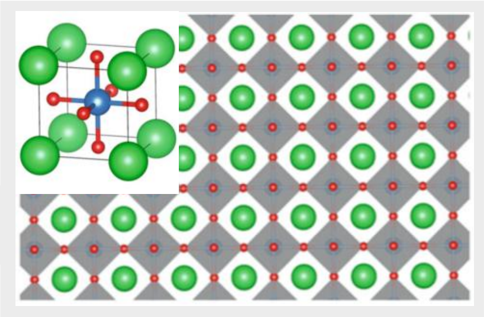
- Perovskite lattice parameter formula based on ionic radii (empirical)
- Lattice parameters range between 3.7 Å and 4.3 Å
  - Maximum lattice parameter mismatch ~ 16%

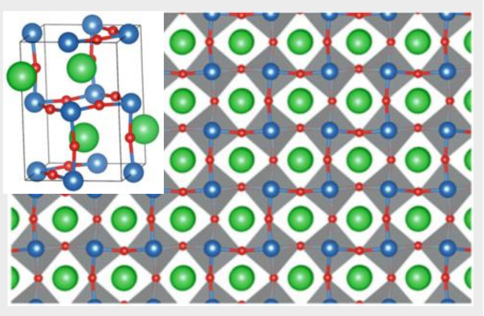
Perovskite oxides

Crystal structures









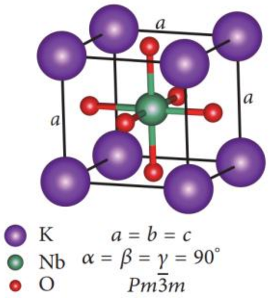
Crystal structure adopted by ABO_3 compounds at room temperature as a function of the ionic radii of the A and B ions for the case divalent A and tetravalent B cations.

public

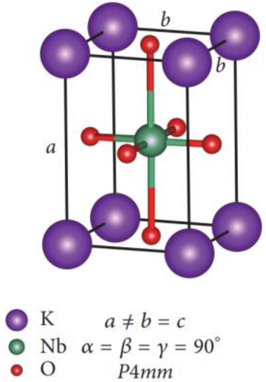
Perovskite oxides

Crystal structures

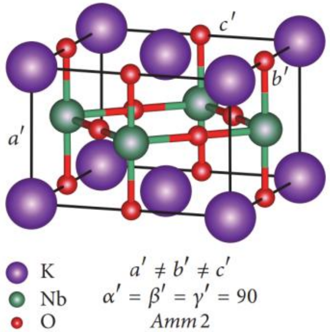
Cubic



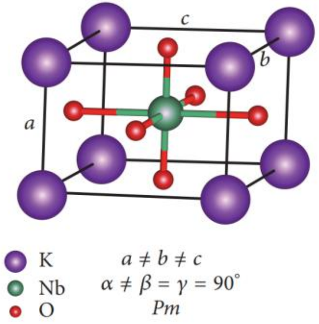
Tetragonal



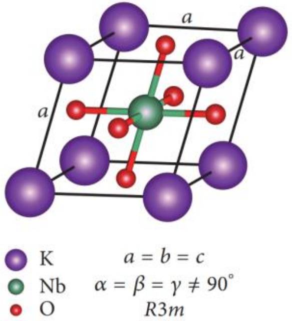
Orthorhombic



Monoclinic



Rhombohedral

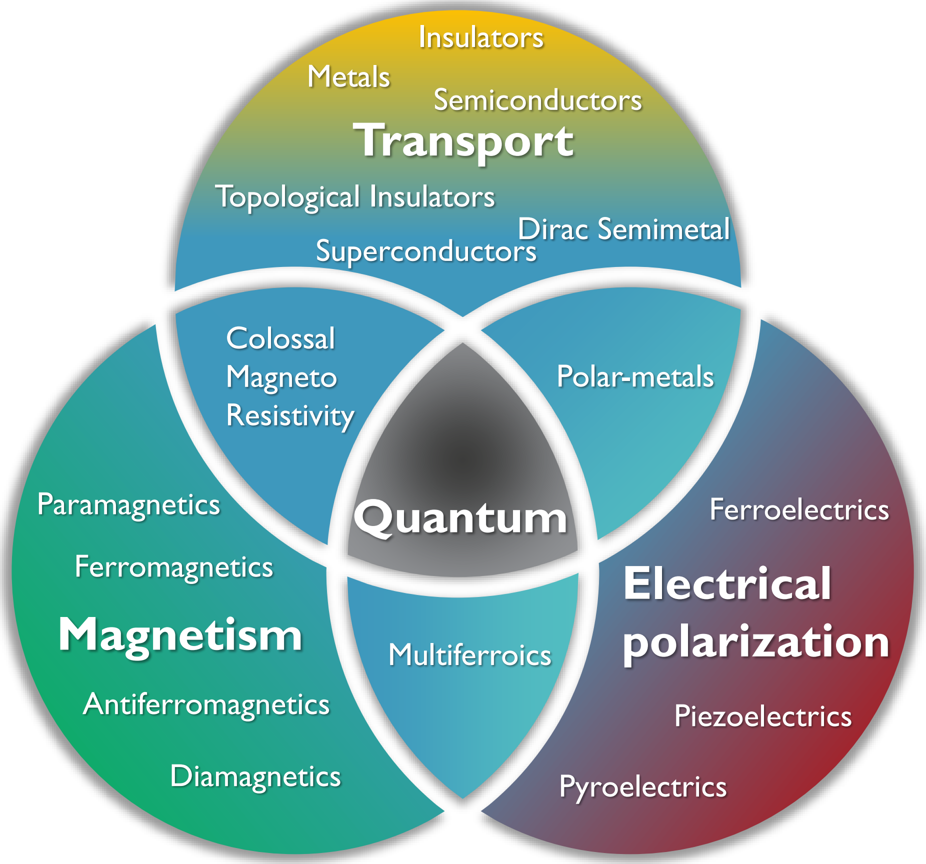


Temperature / Composition / Pressure / Strain / …

Advances in Materials Science and Engineering **39**, 3981317 (2017)
https://doi.org/10.1155/2017/3981317

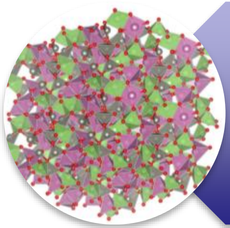
Functional perovskite oxides

- Transport properties
  - Insulator / high-κ: $LaAlO_3$, $SrHfO_3$, $SrZrO_3$
  - Metals: $BaSnO_3$, $LaNiO_3$, $SrRuO_3$
  - Superconductors: $(Ba,K)BiO_3$
  - Topological insulators: $KBiO_3$, $BaBi(O,F)\ _3$
  - Dirac semimetals: $SrIrO_3$
  - Weyl semimetals: $SrRuO_3$
- Electrical polarization properties
  - Piezoelectric: $Pb(Zr,Ti)O_3$
  - Pyroelectric: $(Ba,Sr)TiO_3$
  - Ferroelectric: $BaTiO_3$
- Magnetic properties
  - Ferromagnetic: $(La,Mn)SrO_3$
  - Antiferromagnetic: $(La,Sr)FeO_3$
  - Multiferroic: $BiFeO_3$



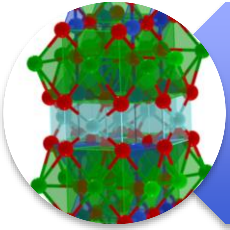
Combination of materials with various properties but with “similar” structures

Exploratory oxides properties



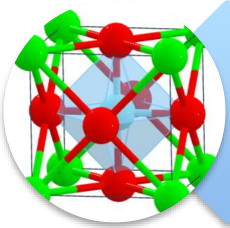
(Semi)conducting

Logic
Memory



Superconducting

Quantum Computing



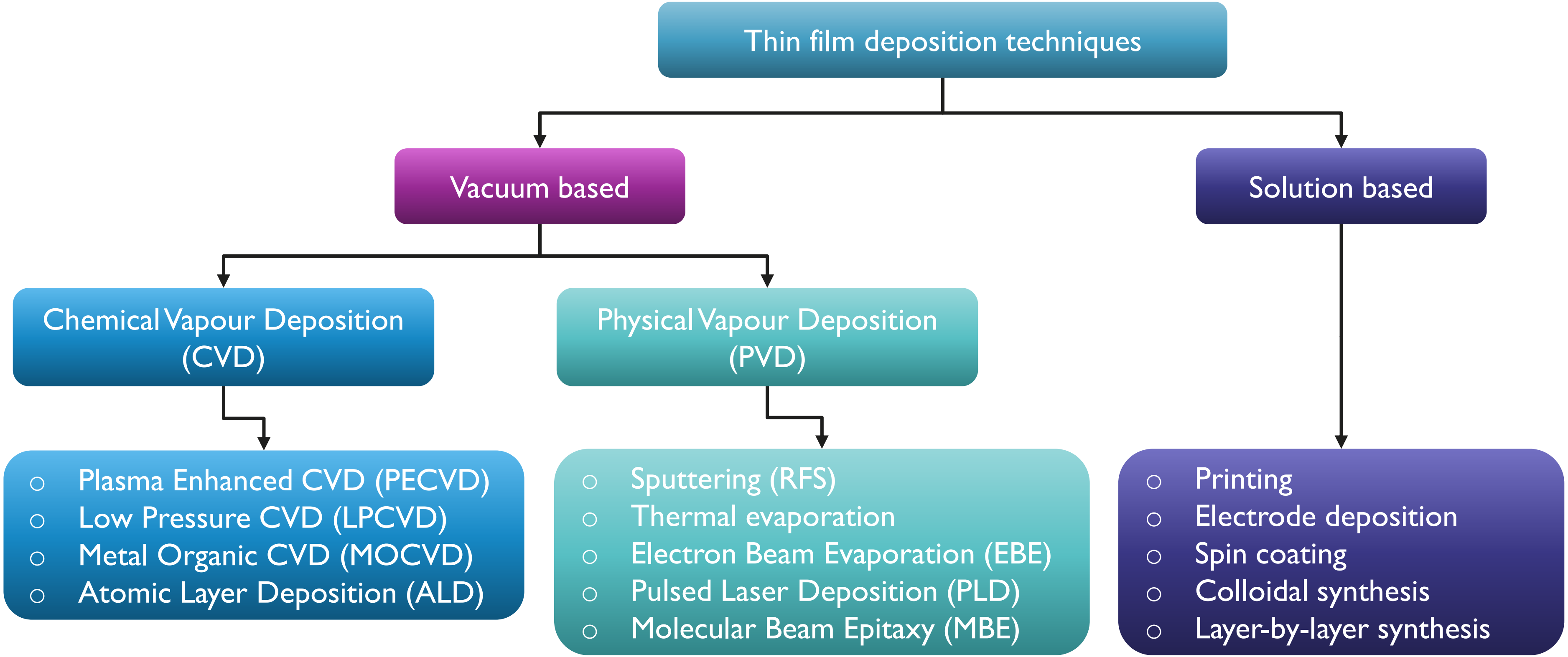
Electro-optical

Optical Interconnect
Quantum Communication
Display & holography

Oxides growth techniques

Metal-oxides deposition methods

Overview



Thin film deposition techniques

Vacuum based

Solution based

Chemical Vapour Deposition (CVD)

Physical Vapour Deposition (PVD)

- Plasma Enhanced CVD (PECVD)
- Low Pressure CVD (LPCVD)
- Metal Organic CVD (MOCVD)
- Atomic Layer Deposition (ALD)

- Sputtering (RFS)
- Thermal evaporation
- Electron Beam Evaporation (EBE)
- Pulsed Laser Deposition (PLD)
- Molecular Beam Epitaxy (MBE)

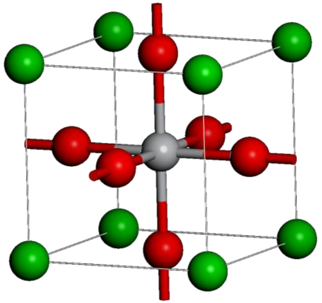
- Printing
- Electrode deposition
- Spin coating
- Colloidal synthesis
- Layer-by-layer synthesis

Epitaxial oxide challenges

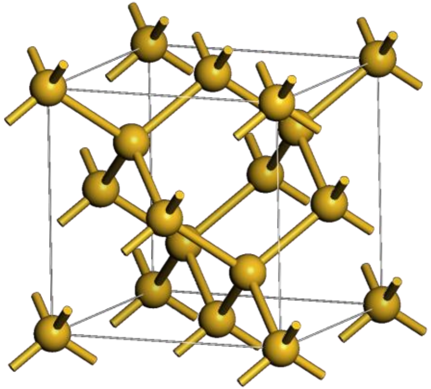
ABO_3 vs. Si

- **Crystal structure** mismatch
  - Perovskite vs. Diamond

Perovskite (ABO_3)

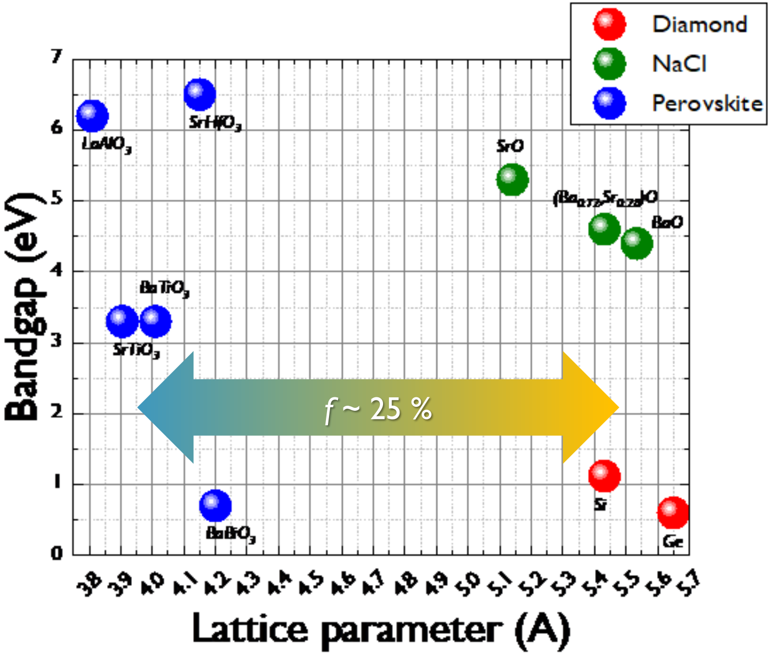


Diamond



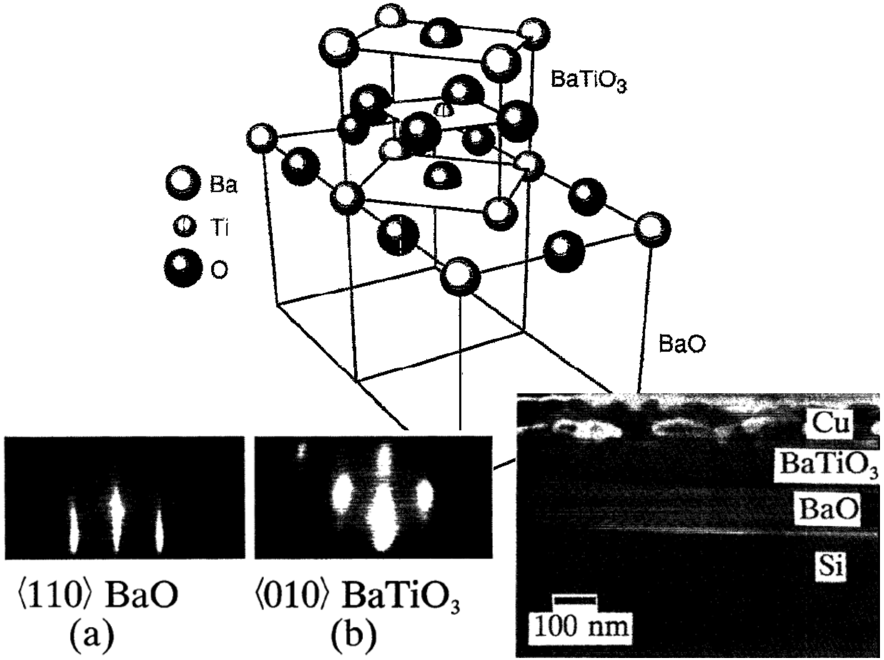
- **Chemical bonding** mismatch
  - Ionic bonds vs. Covalent bonds

- **Lattice parameter** mismatch



Pioneering work

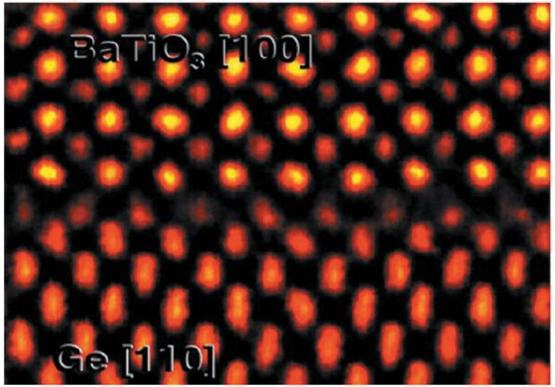
McKee et al., Oak Ridge Univ. (1990 ~ 2000)



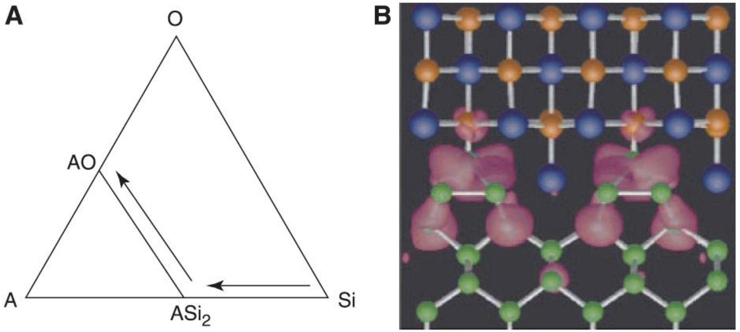
⟨110⟩ BaO
(a)

⟨010⟩ BaTiO$_3$
(b)

Appl. Phys. Lett. **59**, 782 (1991)



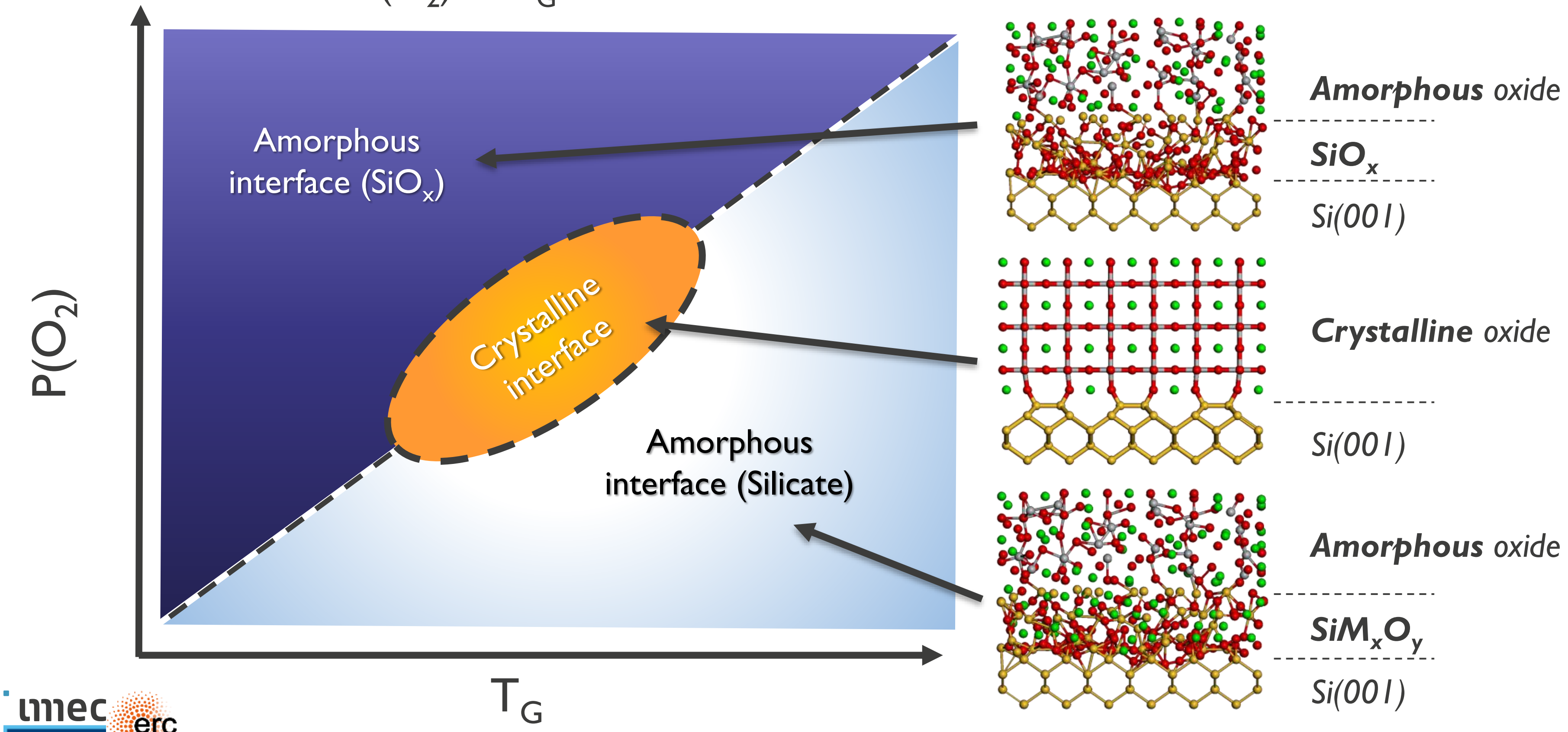
Science 293, 468 (2001)



Science 300, 1726 (2003)

Epitaxial oxide challenges

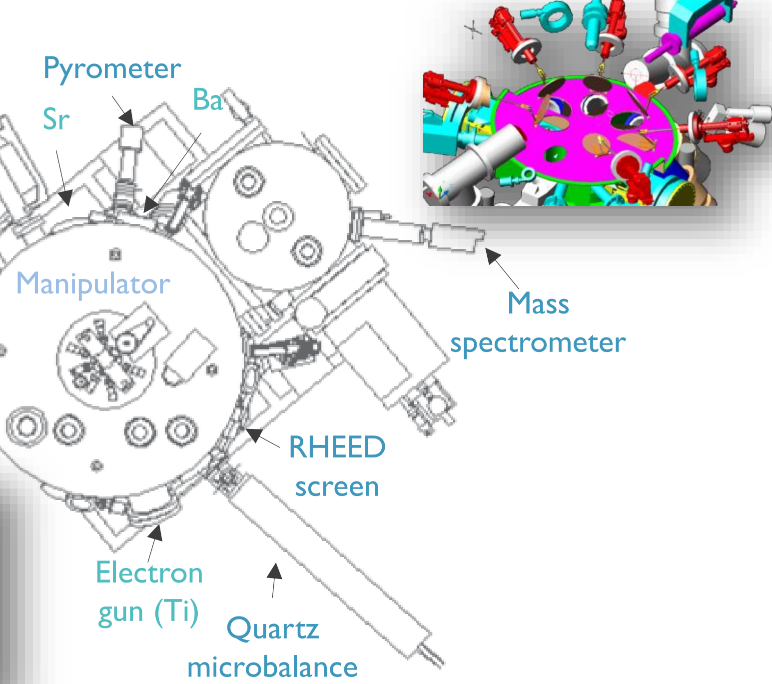
Si interface control: $P(O_2)$ vs. T_G

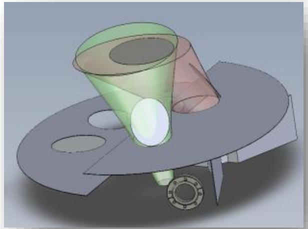


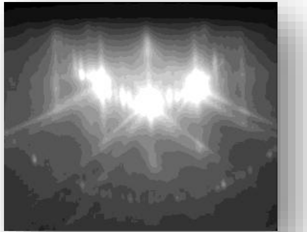
Epitaxial Strategy

Molecular Beam Epitaxy

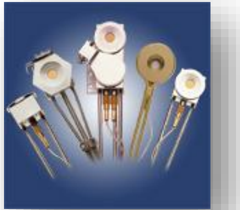
- In-situ analysis growth technique
- Precise flux controlling at atomic level
- Interface engineering
- Tools @ imec
  - 2” to 12” substrates
  - Effusion cells & E-beam
  - Remote plasma sources
  - *in-situ* characterizations
    - RHEED
      - Crystalline state





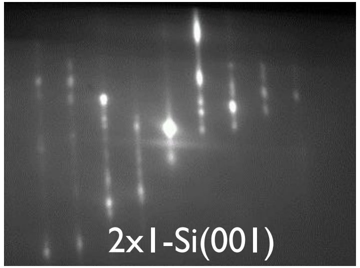


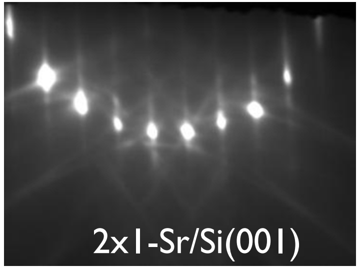
- In-situ quartz microbalance
  - Flow rate calibration



- Mass spectrometers (x6)
  - Evaporation control

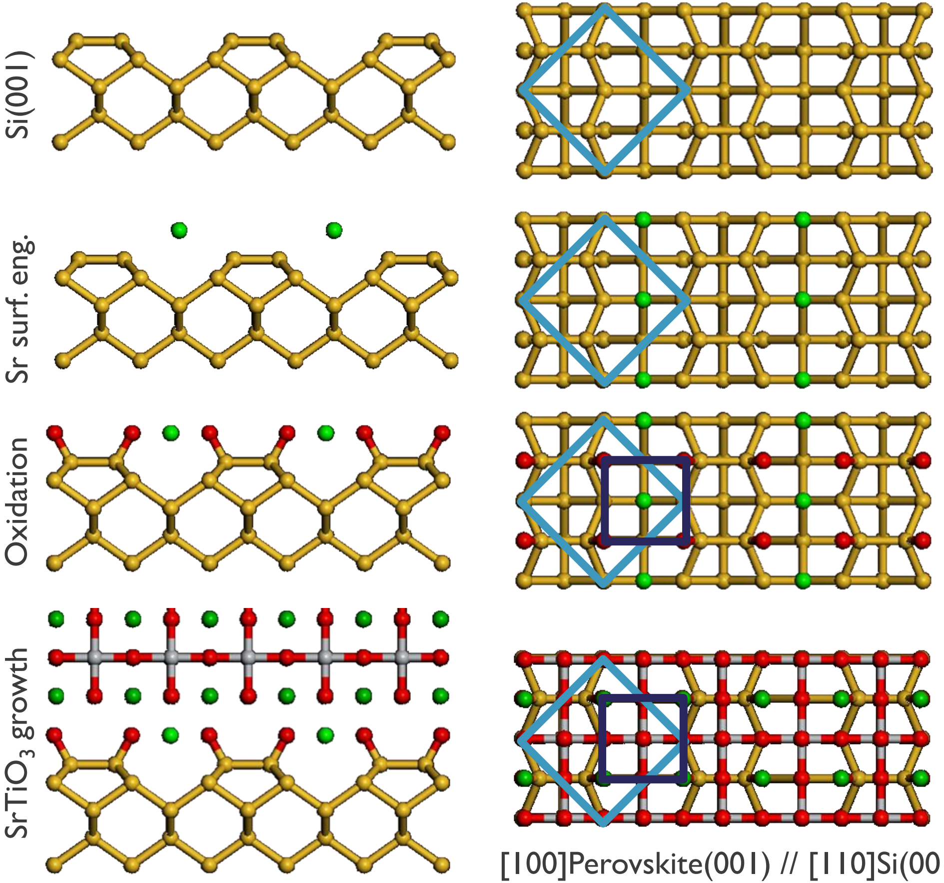
½ ML Sr Submonolayer engineering of Si(001)





Dimerized Si(001) surface

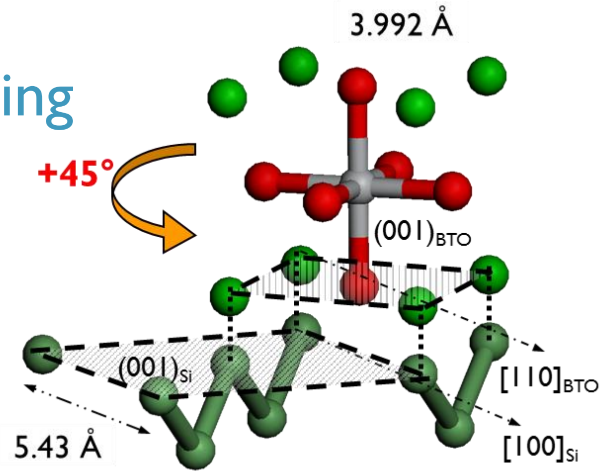
½ ML Sr-Terminated Surface



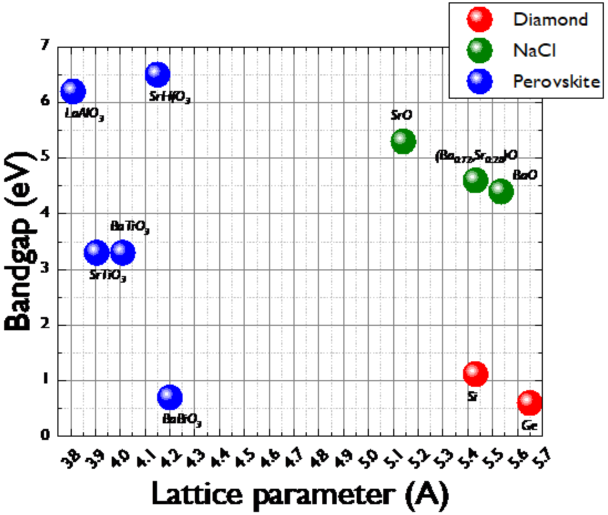
[100]Perovskite(001) // [110]Si(001)

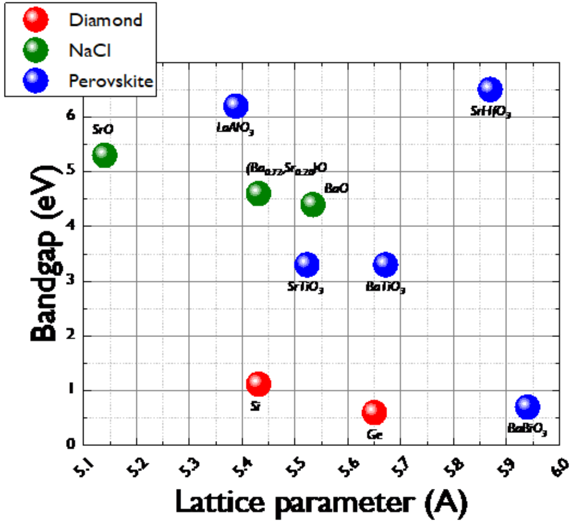
Epitaxial Strategy: Oxide/Si Interface Engineering

Alkaline Submonolayer

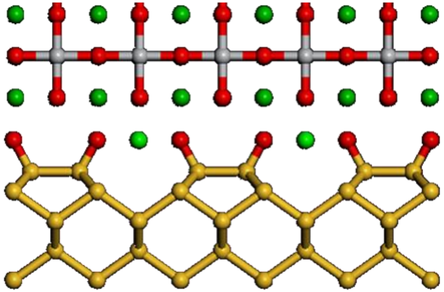


- Alkaline Submonolayer (Mg, Ca, Sr, …)
  - Oxidation Barrier: stable "Si – O – Alkaline" interface
  - Crystal Template: 45° Lattice rotation
  - [100]Perovskite(001) // [110]Si(001)
    - Effective lattice mismatch reduction

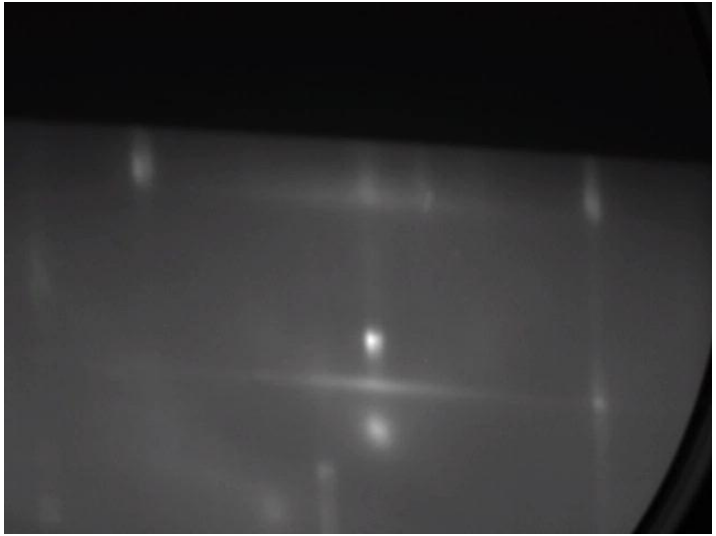




$SrTiO_3$ buffer: the trick ….



- Different strategies for STO growth on Si
  - 2 steps: LT deposition + recrystallization
  - Different buffers: ½ ML SrO -> few nm (Ba,Sr)O
  - Direct STO epitaxy onto Sr-Si(001)

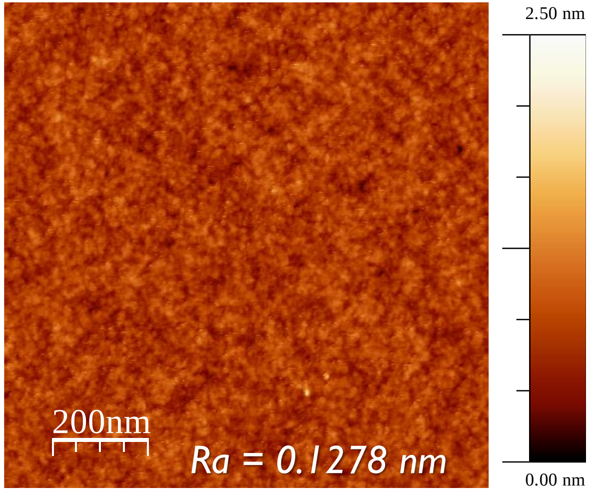


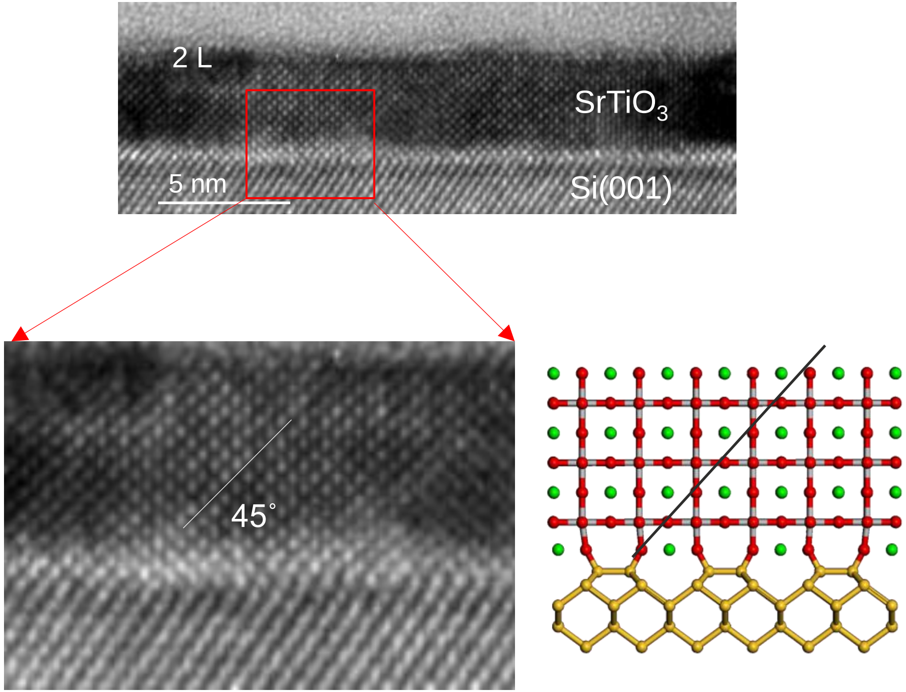
- @ imec: direct STO epitaxy onto Sr-Si(001)
  - T_G ~ 300 C & $P(O_2)$ < 2e-7 Torr
  - Smooth "Si-to-STO" transition by RHEED
  - Strong streak diffractions lines from STO at early stage without amorphization step

High Quality $SrTiO_3$

Low temperature epitaxy on Sr-Si(001)

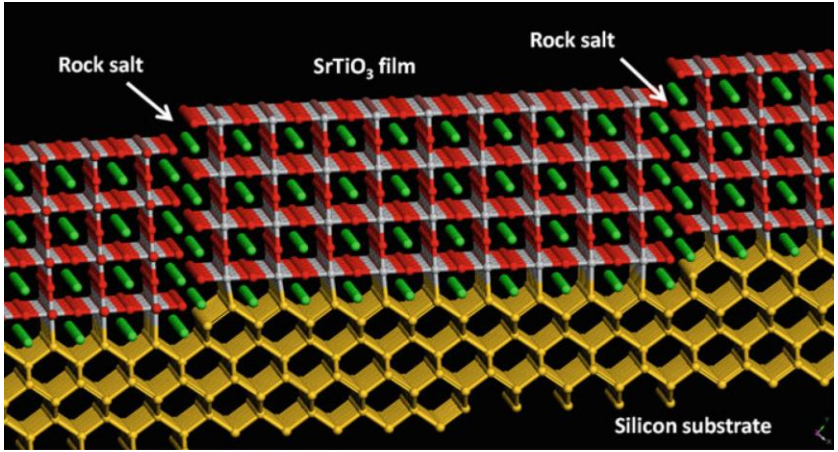
- Excellent STO pseudo-substrate quality for functional oxides integration on Silicon
  - RMS < 0.2 nm
  - Sharp Si/STO interface



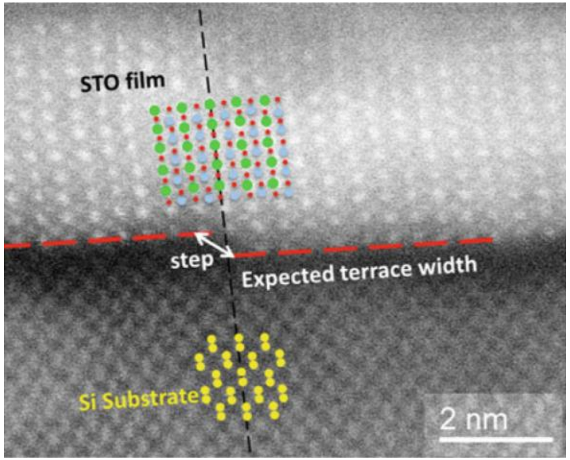


Defects in perovskites

Anti-phase domains



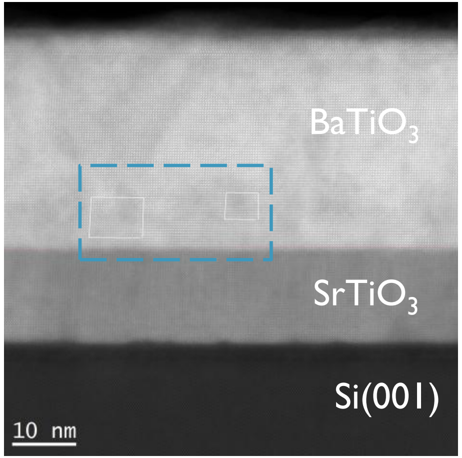
Domain walls at step edges can be healed using the formation of quasi Ruddlesden-Popper layers

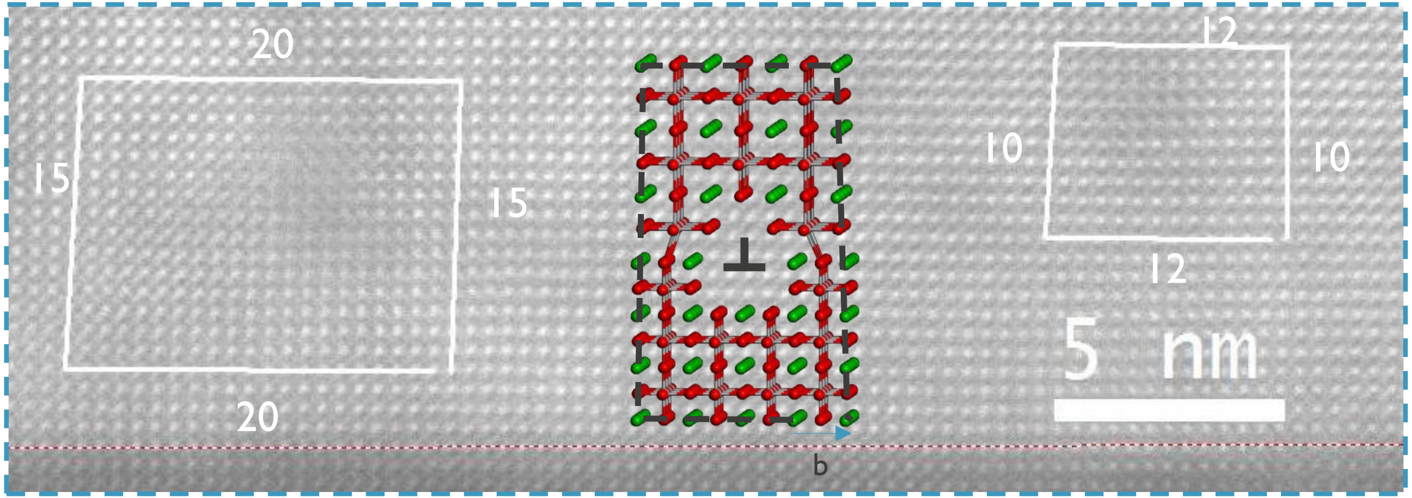


Scanning transmission electron micrograph of STO grown on 4º miscut vicinal Si(100). (Image courtesy of D. J. Smith).

Defects in perovskites

Misfit dislocations



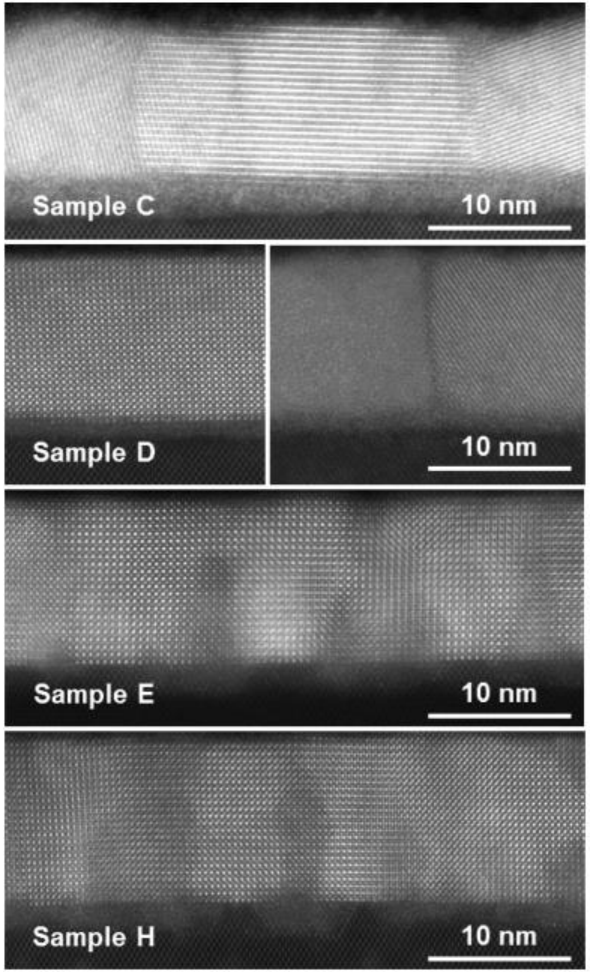


- Strain relaxation via misfit dislocations
- Edge dislocations
  - Burger vector: b = $a_{BTO}\langle 100\rangle$ = 3.995 A

Defects in perovskites

Importance of stoichiometry

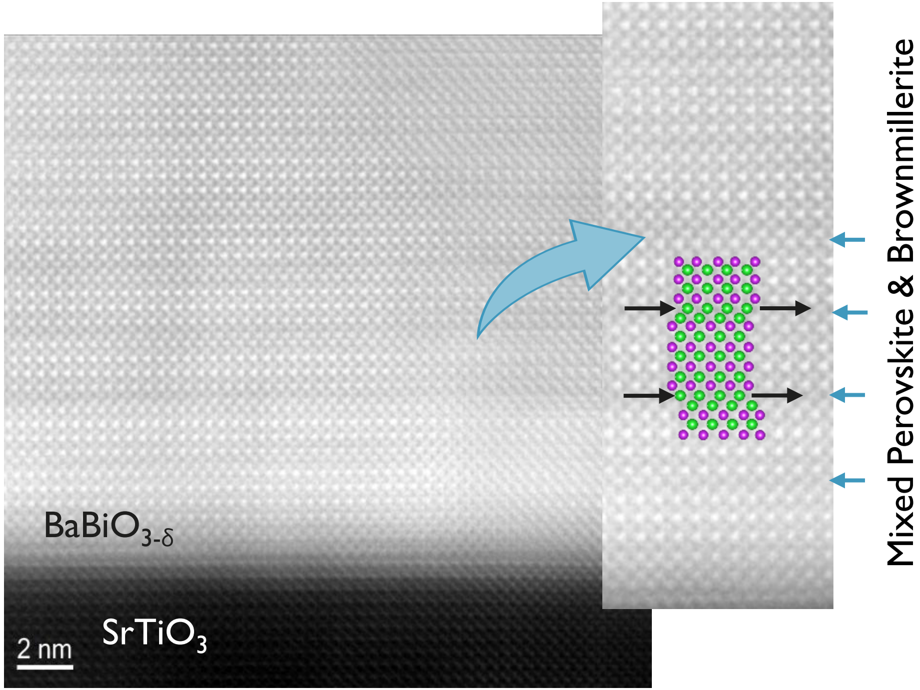
- The Sr/Ti stoichiometry in crucial, any slight variation would drastically influence the layer crystallinity and generate high defect density or amorphous / polycrystalline phases.

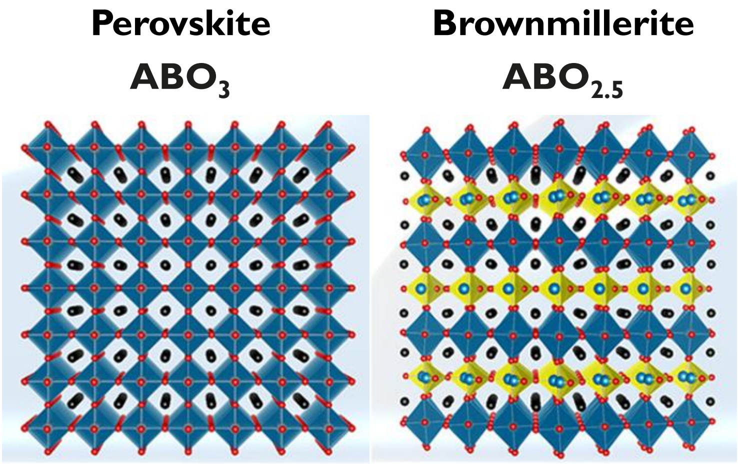


G. Saint Girons et al., Chem. Mater. 2016, 28, 5347−5355

Crystal structure of $BaBiO_{3-\delta}$

HAADF-STEM analysis



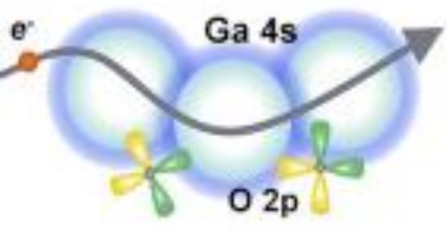


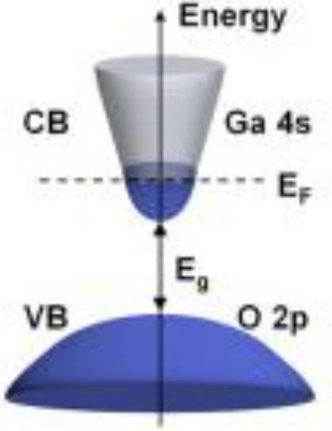
Han, Hyeon, et al., *ACS nano* 16.4 (2022): 6206-6214

- Brownmillerite inclusions
  - Insertion of AO-like planes observed along thin-film's [001] crystallographic direction
- Layered perovskite structure
  - $Ba_2Bi_2O_5$ stoichiometry

[1] I. Ahmed et al., APL Materials 12, 031105 (2024)

Novel applications





Transparent Conducting Oxides

Courtesy of imec (2024)

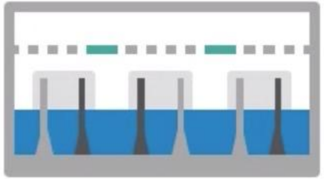
Logic scaling roadmap

3nm
PP:44-48, MP: 21-24

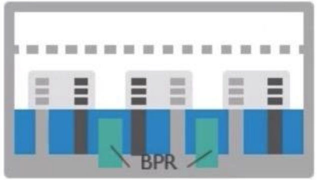
2nm
PP:40-44, MP: 18-21

1.5nm
PP: 40-44, MP: 18-21

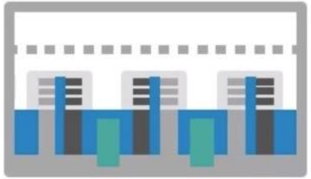
1nm and beyond
PP: 38-42, MP: 15-18



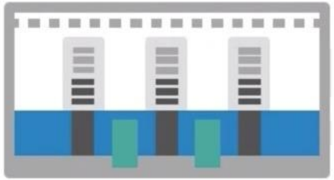
FinFET
5T



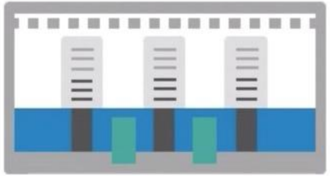
Nanosheets, BPR
5T



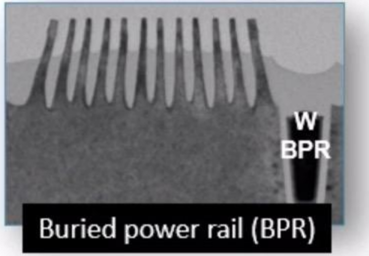
Forksheets, VHV std cell arch.
<5T



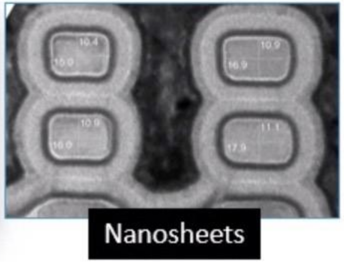
CFET, BEOL w/ airgaps
4T



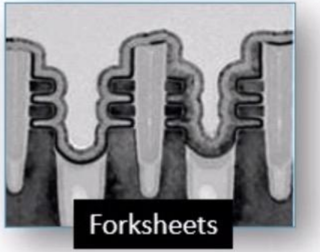
2D atomic channels
<4T



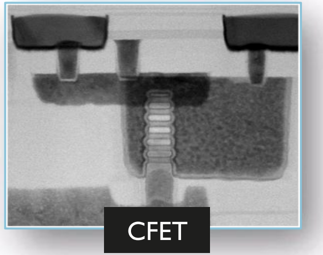
Buried power rail (BPR)



Nanosheets



Forksheets



CFET

WS_2 2D channel FET

Courtesy of imec (2024)

Interconnect scaling roadmap

Dual damascene
iN7, iN5, iN3?

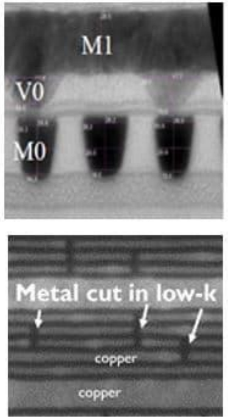
Supervia
iN3 and beyond

Semi-damascene
iN3 and beyond

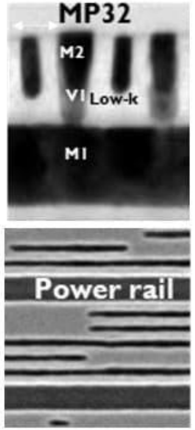
Adding functionality

New conductor

multipatterning

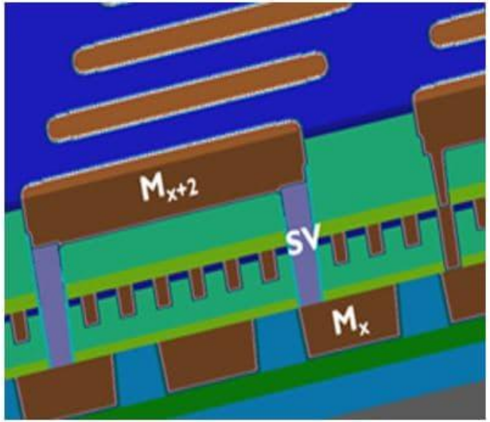


EUV single print



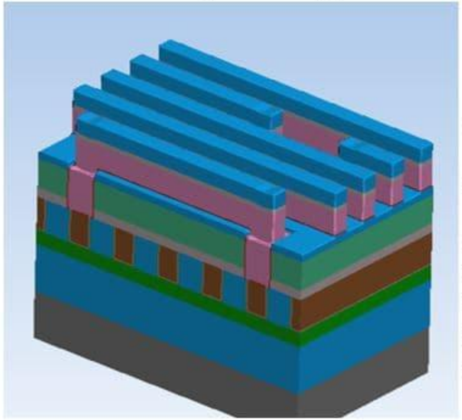
Conventional dual damascene reference

High aspect ratio supervia



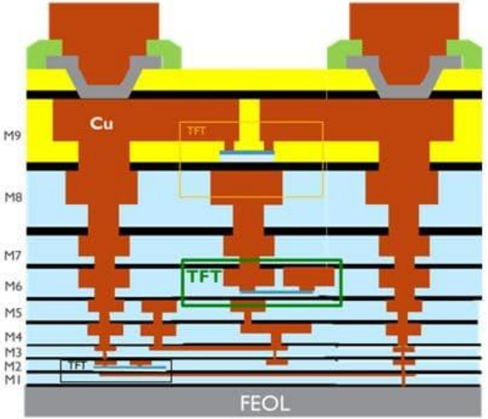
Extension for better routability

Metal patterning



Barrierless AG module for overcoming RC

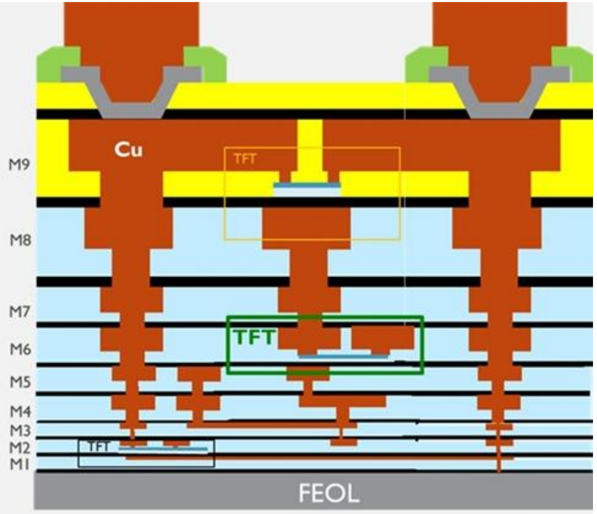
Thin Film Transistor in BEOL

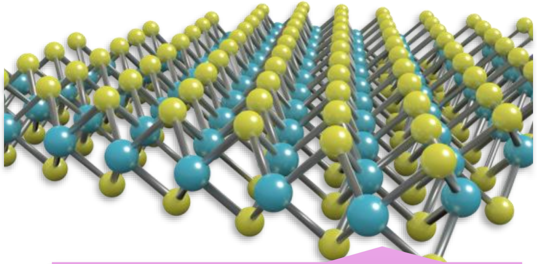


Power gating, repeaters, memory

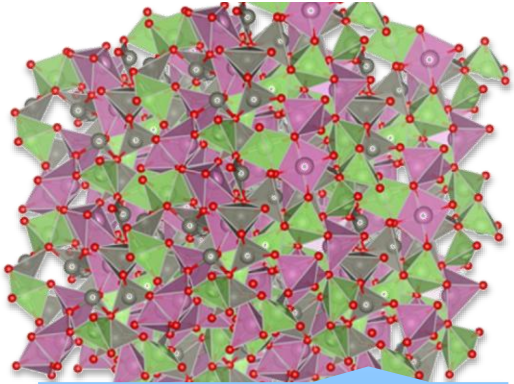
BEOL/MOL transistors & selectors

Vertical scaling

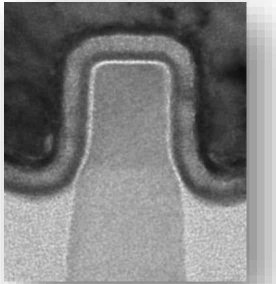




2D materials (TMDs)



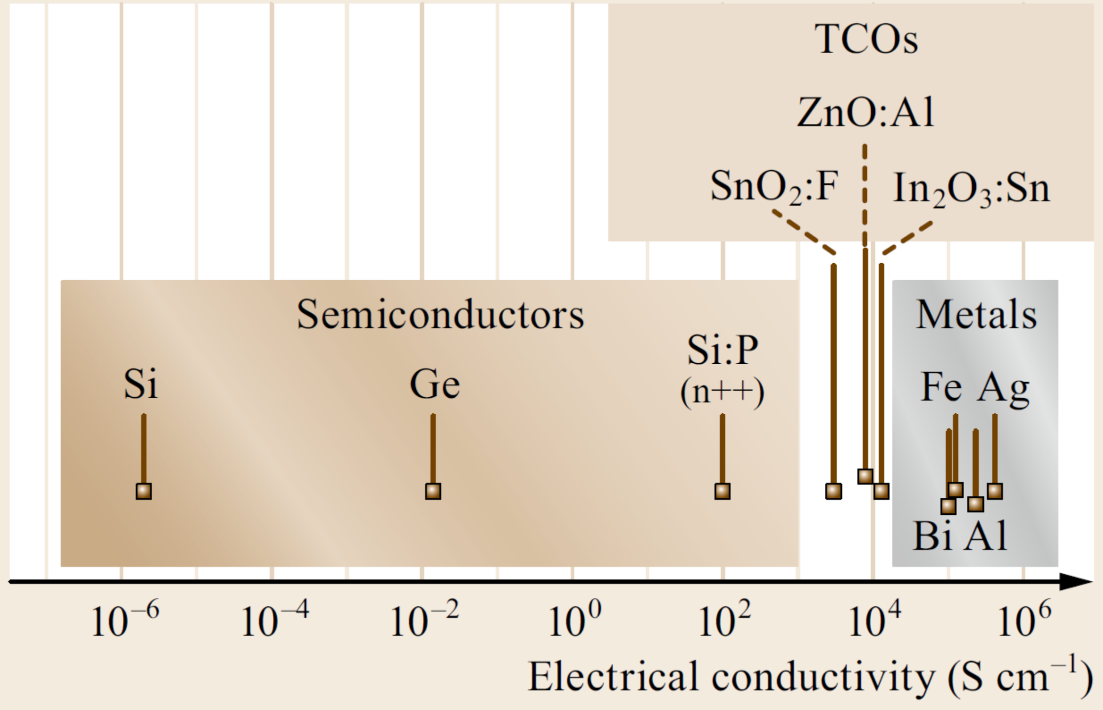
Trans. Cond. Oxides (TCOs)



- Temperature limitation: BEOL < 400°C
- Mobility > 50 $cm^2V^{-1}s^{-1}$
- n- & p-type conductivities

Transparent Conductive Oxides (TCO)

Degenerate semiconductors / transparent metal

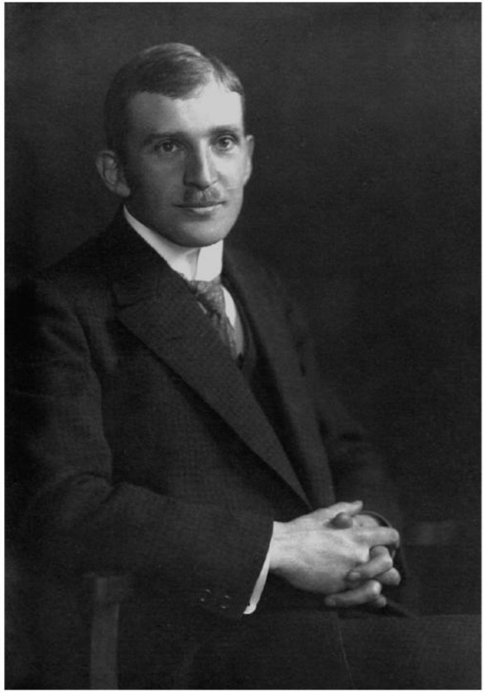


- Conductivity of TCO resides between semiconductors and metals
- Properties of TCO
  - Wide bandgap (>2.5 eV)
  - High conductivity
  - Low absorption and reflection of light
  - Doping

Transparent Conductive Oxides (TCO)

History of inventions: starting with CdO

First mention of conducting CdO crystal:
F. Streintz, Ann. Phys. 9, 854 (1902)



Karl Bädeker: discoverer of conducting thin film CdO

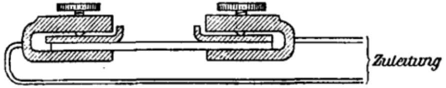


Fig. 1.

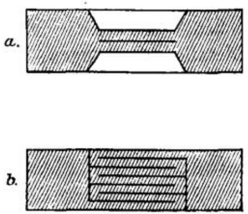


Fig. 2.

Resistivity measurement on CdO samples in the 'early days'

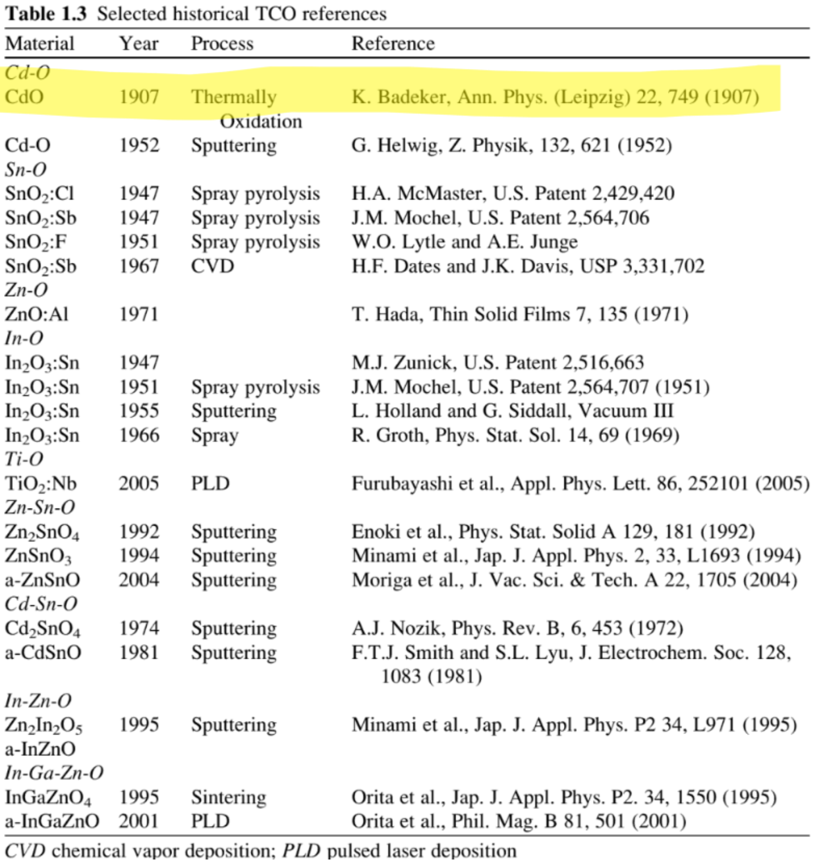


Table 1.3 Selected historical TCO references

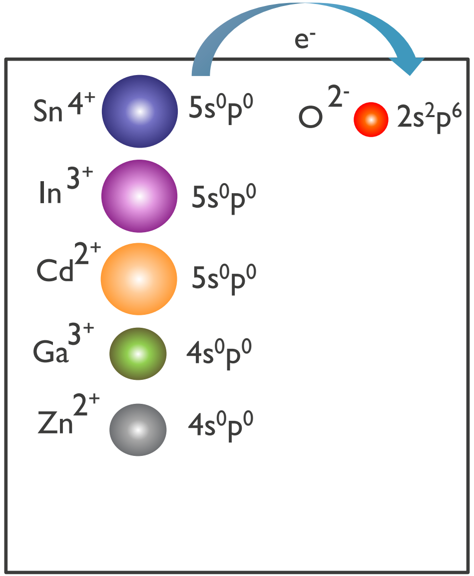
Material	Year	Process	Reference
Cd-O			
CdO	1907	Thermally Oxidation	K. Badeker, Ann. Phys. (Leipzig) 22, 749 (1907)
Cd-O	1952	Sputtering	G. Helwig, Z. Physik, 132, 621 (1952)
Sn-O			
SnO_2:Cl	1947	Spray pyrolysis	H.A. McMaster, U.S. Patent 2,429,420
SnO_2:Sb	1947	Spray pyrolysis	J.M. Mochel, U.S. Patent 2,564,706
SnO_2:F	1951	Spray pyrolysis	W.O. Lytle and A.E. Junge
SnO_2:Sb	1967	CVD	H.F. Dates and J.K. Davis, USP 3,331,702
Zn-O			
ZnO:Al	1971		T. Hada, Thin Solid Films 7, 135 (1971)
In-O			
In_2O_3:Sn	1947		M.J. Zunick, U.S. Patent 2,516,663
In_2O_3:Sn	1951	Spray pyrolysis	J.M. Mochel, U.S. Patent 2,564,707 (1951)
In_2O_3:Sn	1955	Sputtering	L. Holland and G. Siddall, Vacuum III
In_2O_3:Sn	1966	Spray	R. Groth, Phys. Stat. Sol. 14, 69 (1969)
Ti-O			
TiO_2:Nb	2005	PLD	Furubayashi et al., Appl. Phys. Lett. 86, 252101 (2005)
Zn-Sn-O			
Zn_2SnO_4	1992	Sputtering	Enoki et al., Phys. Stat. Solid A 129, 181 (1992)
$ZnSnO_3$	1994	Sputtering	Minami et al., Jap. J. Appl. Phys. 2, 33, L1693 (1994)
a-ZnSnO	2004	Sputtering	Moriga et al., J. Vac. Sci. & Tech. A 22, 1705 (2004)
Cd-Sn-O			
Cd_2SnO_4	1974	Sputtering	A.J. Nozik, Phys. Rev. B, 6, 453 (1972)
a-CdSnO	1981	Sputtering	F.T.J. Smith and S.L. Lyu, J. Electrochem. Soc. 128, 1083 (1981)
In-Zn-O			
$Zn_2In_2O_5$	1995	Sputtering	Minami et al., Jap. J. Appl. Phys. P2 34, L971 (1995)
a-InZnO			
In-Ga-Zn-O			
$InGaZnO_4$	1995	Sintering	Orita et al., Jap. J. Appl. Phys. P2. 34, 1550 (1995)
a-InGaZnO	2001	PLD	Orita et al., Phil. Mag. B 81, 501 (2001)

CVD chemical vapor deposition; *PLD* pulsed laser deposition

Courtesy of Harold Dekkers - imec (2024)

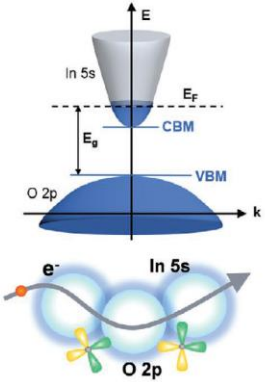
Polar/Ionic binding

Formation of conduction band

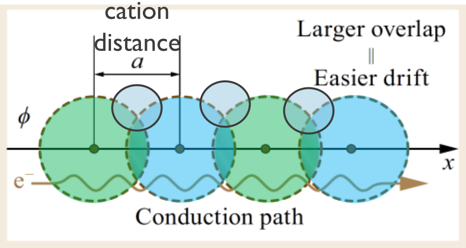


Ionic balance:

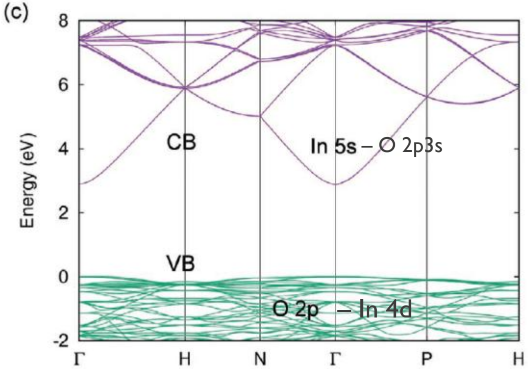
Metals transfer electrons to oxygen
Metal *s*-orbitals are empty
overlaps forming conduction band



s-orbitals are spheres: no orientation dependency

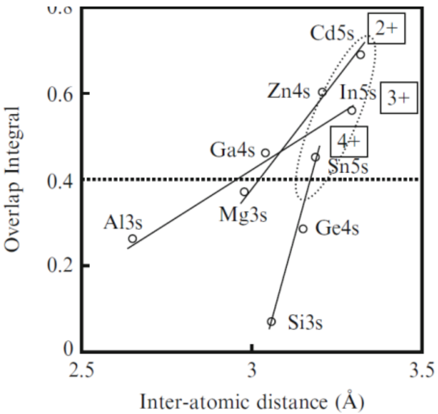


Conduction path improves with orbital overlap

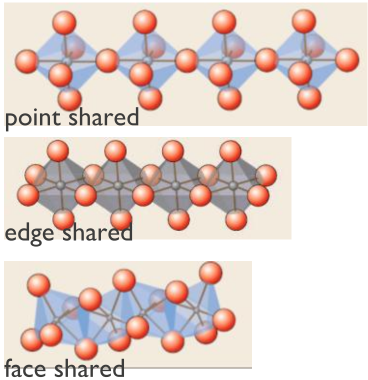


Large overlapping s-orbitals in conduction band: low m_e^* → large electron mobility

O 2p-orbitals: flat band → localized states: very high m_h^* → very low hole mobility



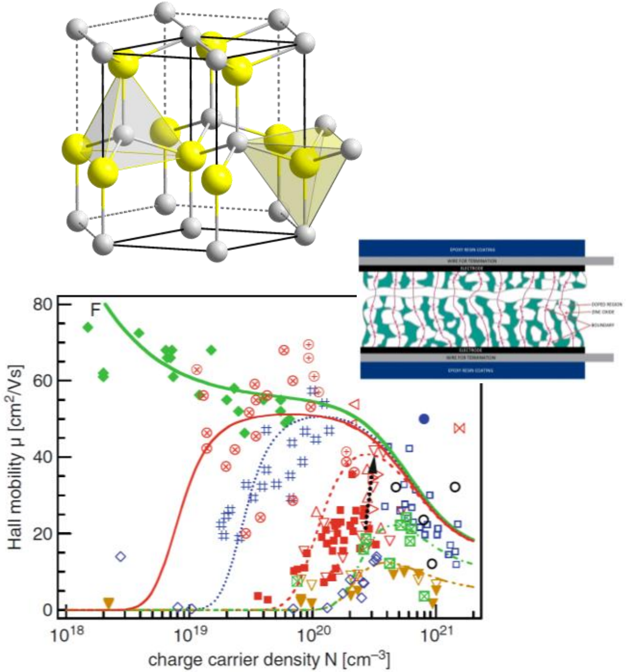
Overlap depends on S-orbital size and atom distance



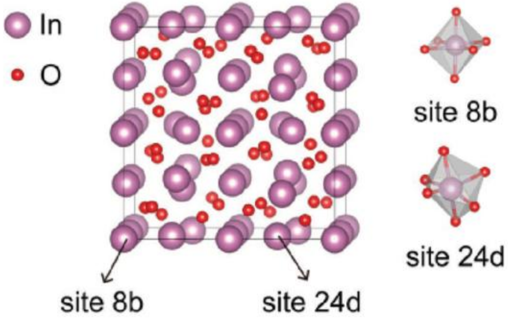
Atom distance depends on morphology (i.e. arrangement of oxygen octahedrals)

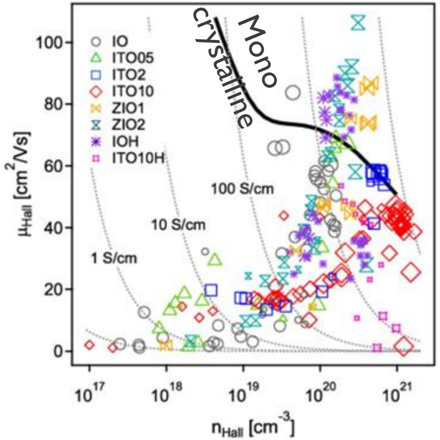
TCOs

ZnO

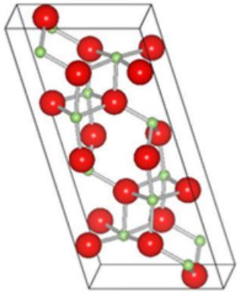


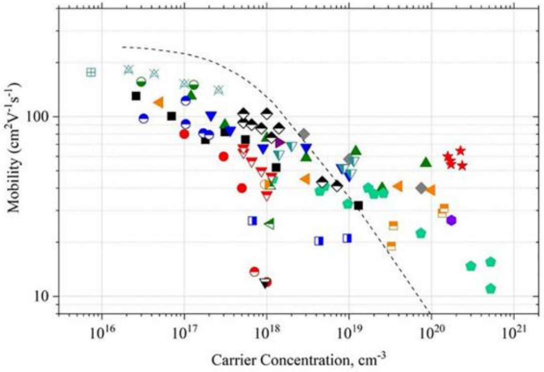
In_2O_3





Ga_2O_3



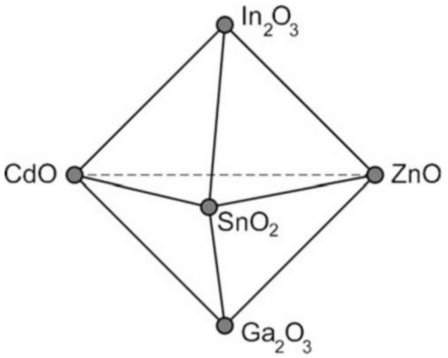


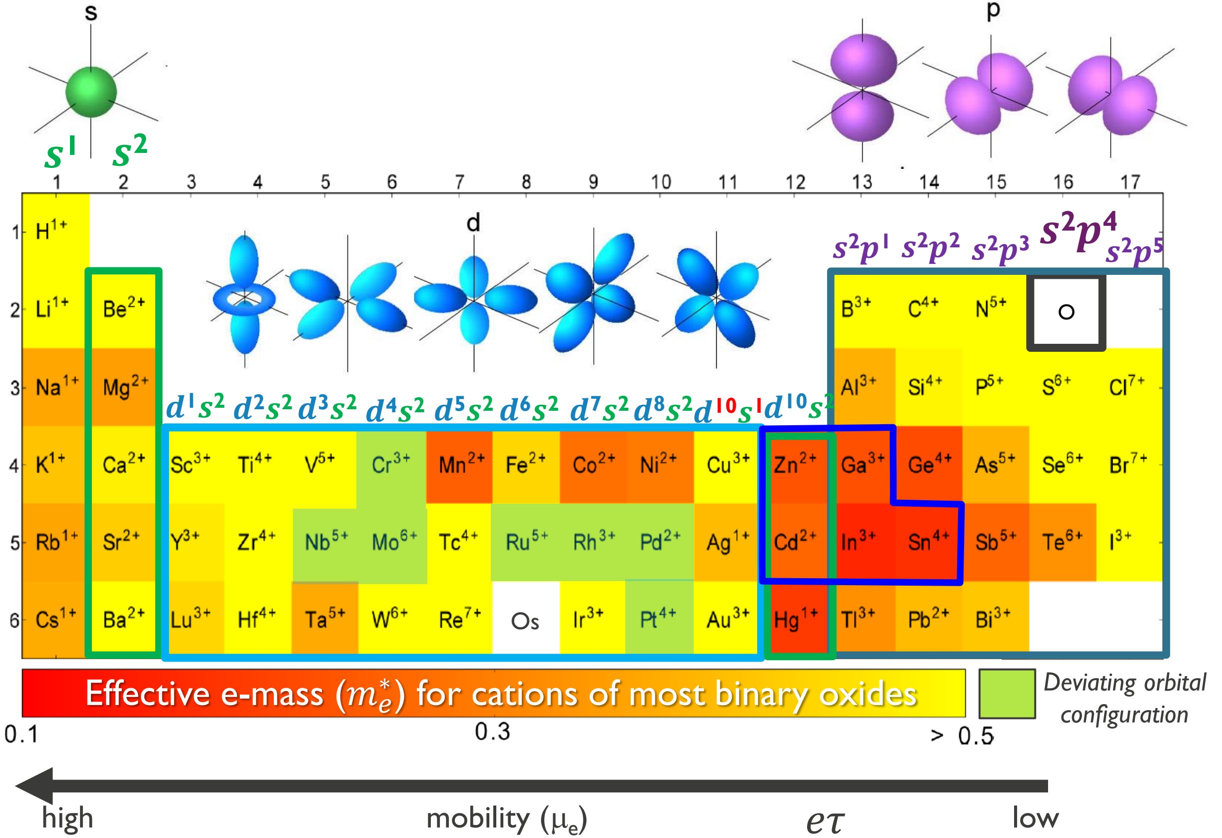
Courtesy of Harold Dekkers - imec (2024)

Transparent conductive oxides (TCO)

Material system

- General observations
  - Most stable stoichiometric oxides: always n-type
  - Highest mobilities assigned to oxides with filled d-orbitals (d^{10}) and filled s^2 valence orbitals



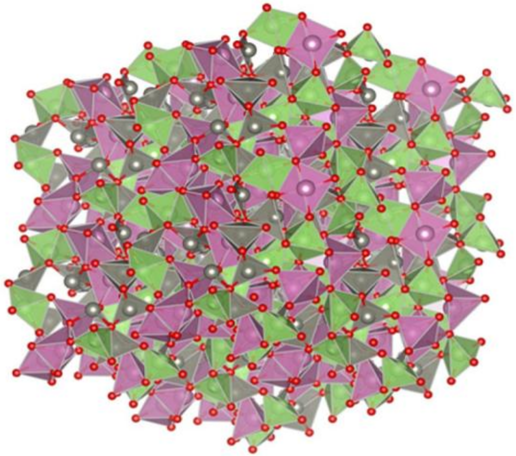


$$\mu_e = \frac{e\tau}{m_e^*}$$

Courtesy of Harold Dekkers - imec (2024)

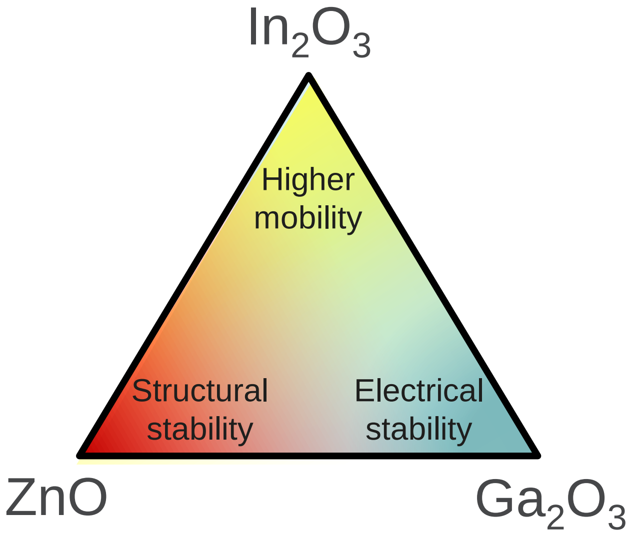
$In_xGa_yZn_zO_4$

Three important aspects



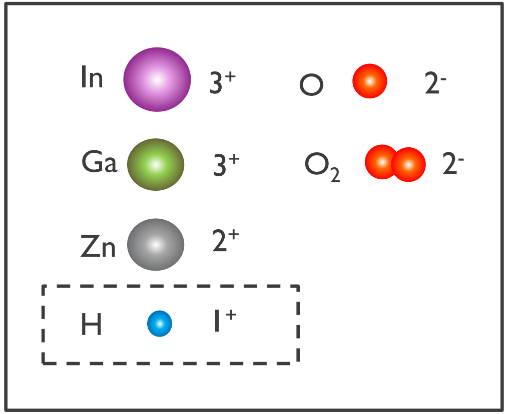
Morphology

- Bonding configuration (only statistical in amorphous)
- Reduced electron mobility by disorder (amorphous)



Compositions

- Properties can be optimized by changing metal composition



Ionic balance

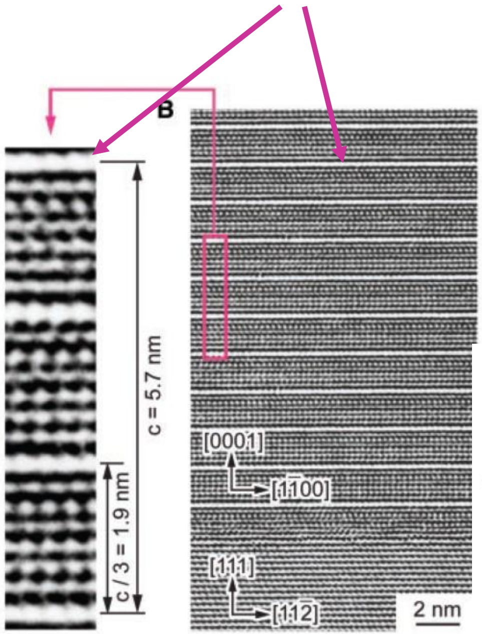
determines doping: density of ***free*** electrons or ‘***frozen’*** holes

Courtesy of Harold Dekkers - imec (2024)

Discovery of IGZO

Monocrystalline IGZO:

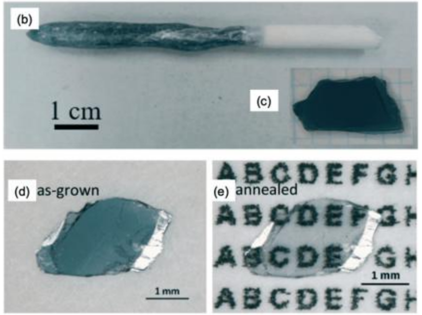
- Intriguing layered structure already known since 1995, grown by PLD or MBE
- First devices in 2004 showed μ_e = 80 cm^2/Vs with **<u>n_e ~10^{14}</u>** cm^{-3}
- High mobility assigned to s-orbitals InO_2 planes
- **Amorphous IGZO** shows similar performance
  - Only 5 × – 8 × lower μ_e (Compare a-Si: 100× lower mobility than c-Si)
  - Keeping n_e under control **<u>n_e ~10^{17} cm^{-3}</u>**



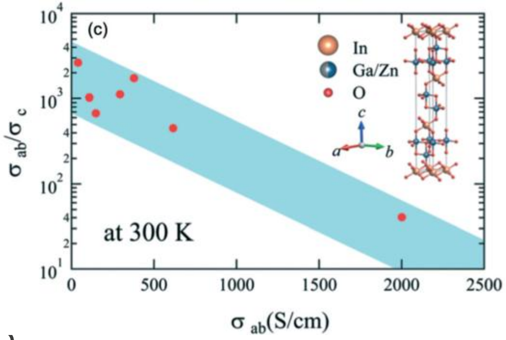
Mobility associated to InO_2 planes

TEM analysis of epitaxial IGZO

N. Kase, Cryst. Eng. Comm , 24, 4481 (2022)



Single crystal IGZO obtained with float zone method



Conductivity of monocrystalline IGZO in direction of InO_2 is remarkably higher

Y. Tanaka.. Eng. Comm, 21, 2985 (2019)

Courtesy of Harold Dekkers - imec (2024)

IGZO TFT in micro-electronics

Using state of the art process from display technology

Advantages

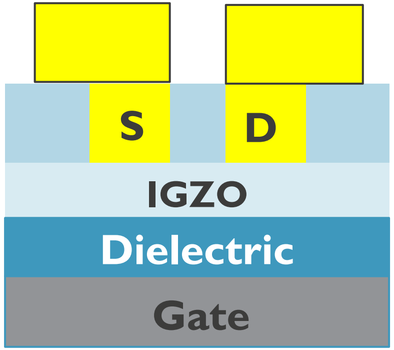
- Low temperature → Application in BEOL
- Relative high mobility (10 – 40 cm²/Vs)
  - Amorphous Si: < 2 cm²/Vs
- Large band gap
- Exclusively n-type

} No minority carriers →

- Accumulation NMOS
- No inversion in off-state
- Simple ‘pinch-off’ FET with low leakage

Challenges

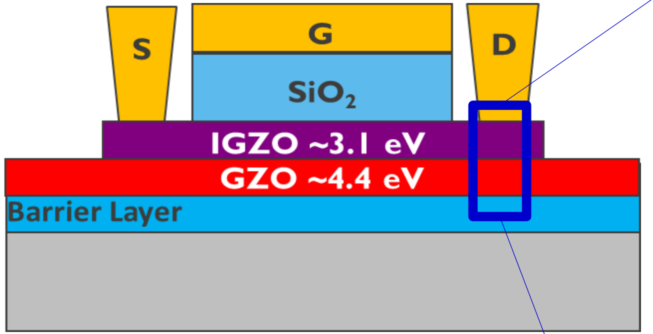
- Establishing 300 mm wafer processing
  - PVD with established IGZO targets
  - ALD conformal deposition
  - Doping: oxygen vacancies & Hydrogen
  - → Sensitive to (process) ambient → Reliability issues

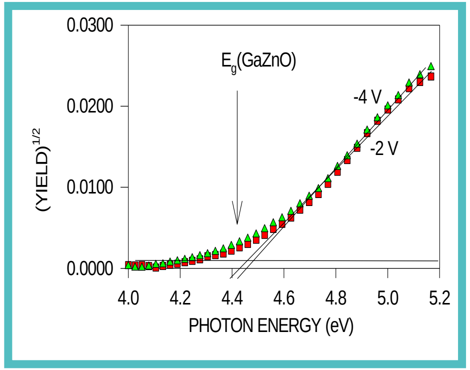


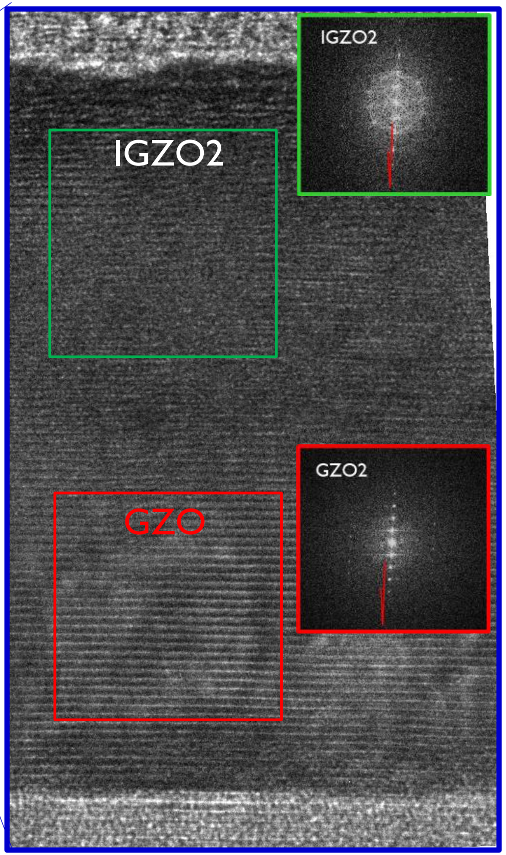
Courtesy of Harold Dekkers - imec (2024)

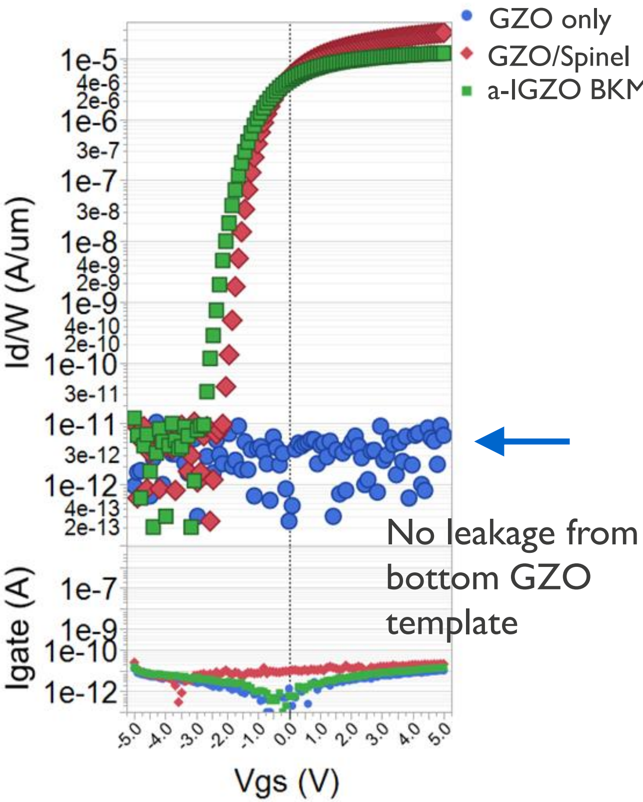
PVD IGZO devices

Realization of pure spinel IGZO









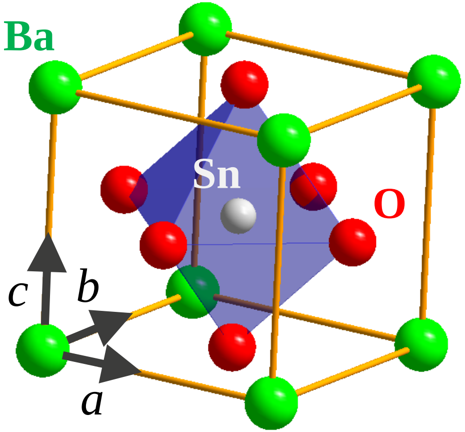
No leakage from bottom GZO template

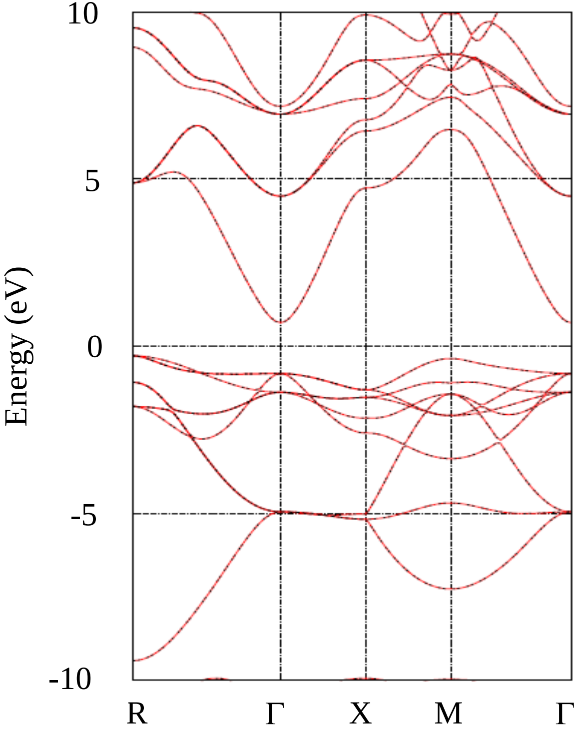
Amorphous GZO crystallizes into spinel at 700 °C and can be used as template for IGZO

Beyond IGZO

$BaSnO_3$ perovskite

Properties	**$BaSnO_3$**
Lattice parameter	4.116 Å
Optical bandgap	3.1 eV



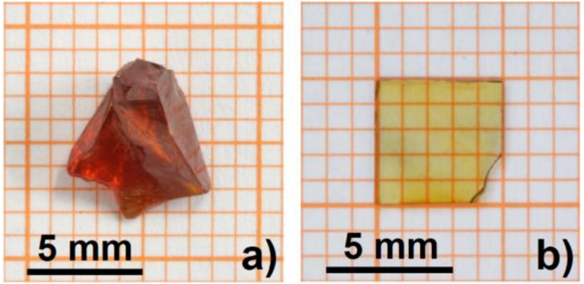


Hiroshi Mizoguchi *et al.*,
Inorg. Chem. **43**, 1667 (2004)

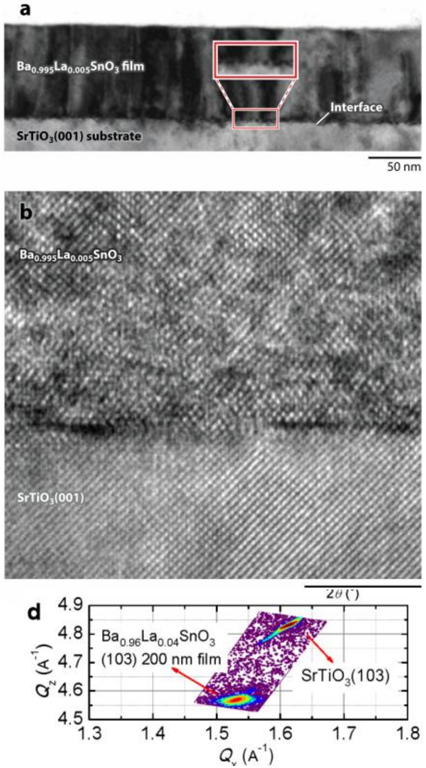
- $BaSnO_3$ can have high mobility intrinsically due to 5*s* orbital of Sn^{4+}
- SnO_6 octahedral network is a main conduction channel.
- There is dopant-site dependency
    - N-doping: Sn4+ site : Sb5+ or Ba2+ site : La3+

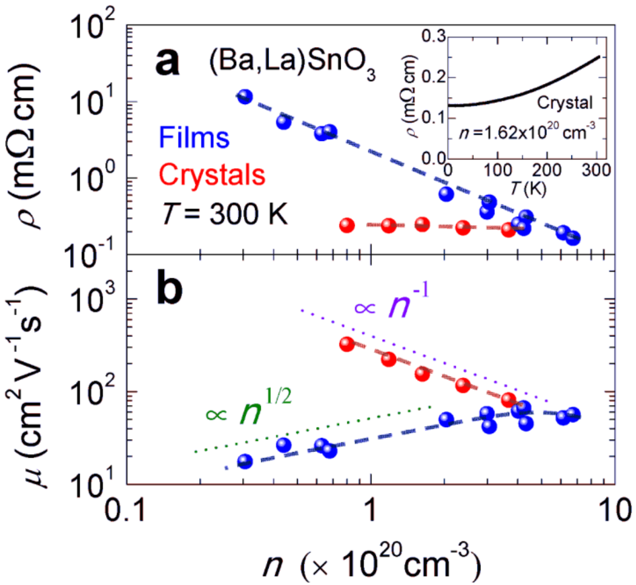
$BaSnO_3$ mobility

Bulk vs. thin films



- In bulk, record mobility of μ = 320 $cm^2.V^{-1}.s^{-1}$ at RT demonstrated
- In thin films, reduced mobility due to scattering via defects (grain boundaries, dislocations, …)
- Lattice matched substrates solution to enhances mobility in films.





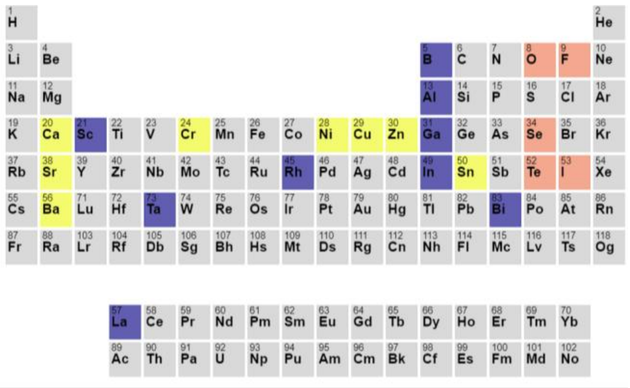
Lee W-J, et al. 2017.
Annu. Rev. Mater. Res. 47:391–423

H. J. Kim *et al.*, Phys. Rev. B **86**, 165205 (2012).
H. J. Kim and U. Kim *et al.*, Appl. Phys. Express **5**, 061102 (2012).

p-type TCOs

Data mining

Chemical space > 60 literature reports

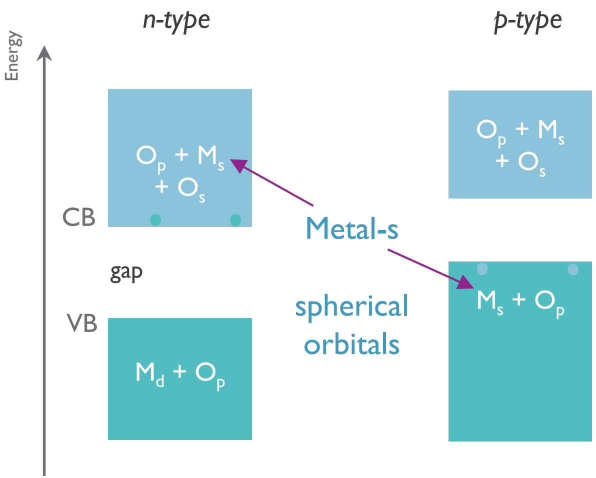


Anion

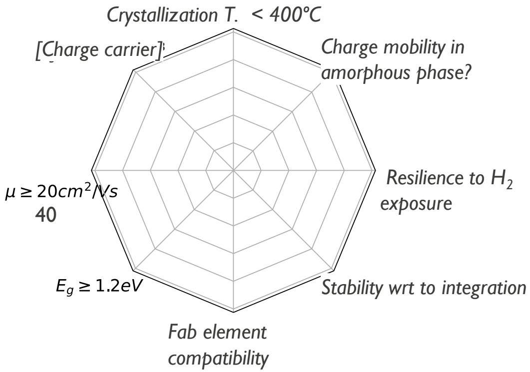
Cation: alloy stabilizing elements

Cation: s orbital in the valence band for transport

Electronic structure



Material profile



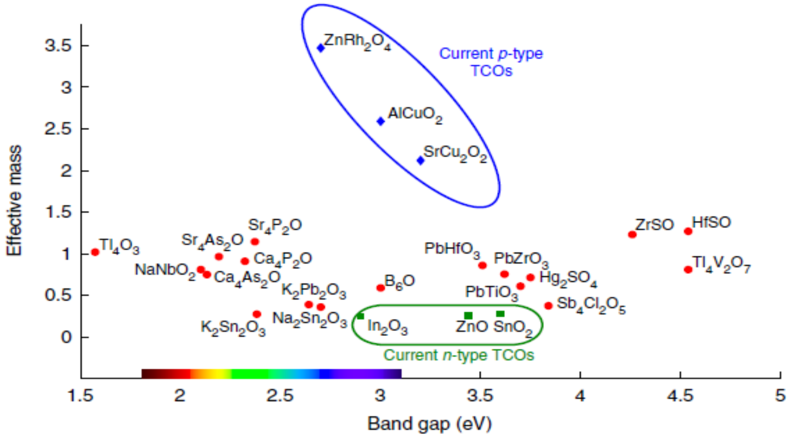
Challenges:

- p-type mobility depends on the presence of metal s orbitals in the valence band → Cu,Zn,Sr,... based oxides
- Doping = defects
- Current reported p-type = crystalline phases

p-Type TCOs

Ab-initio

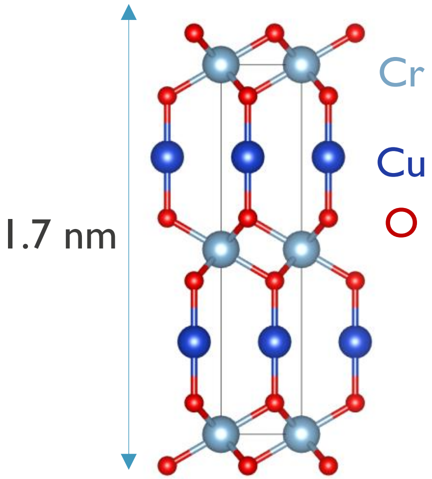
Crystalline oxide



Effective mass versus band gap for the p-type TCO candidates.

Geoffroy Hautier et al , NATURE COMMUNICATIONS | 4:2292 | DOI: 10.1038/ncomms3292 (2013)

CuCrO$_2$ delafossite
Quasi-2D semiconductor



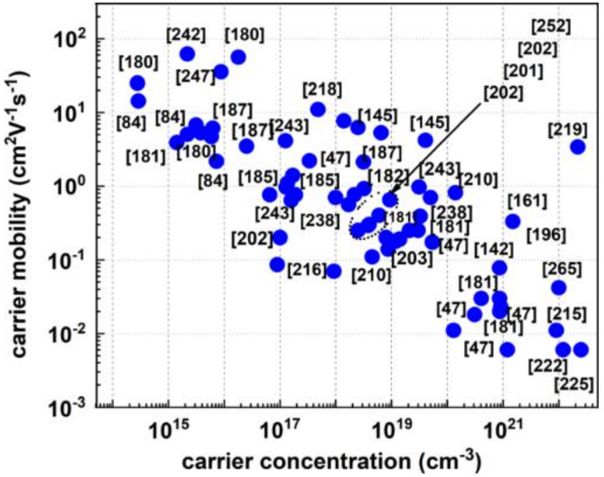
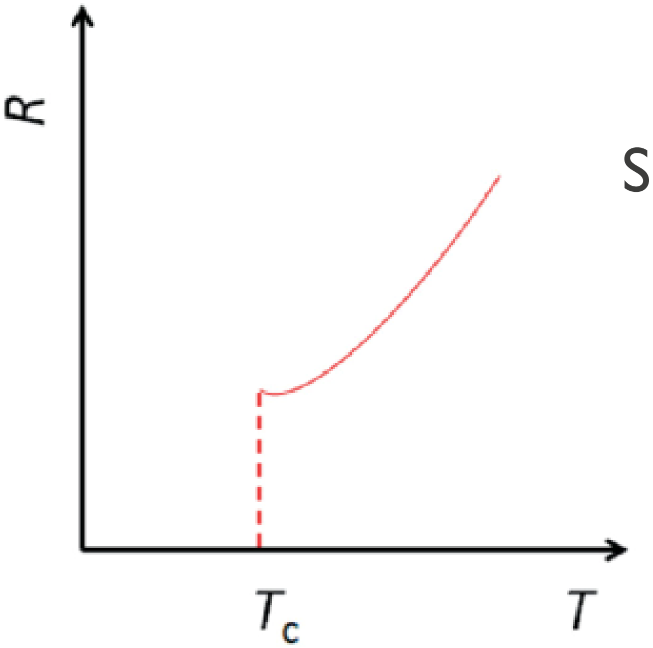


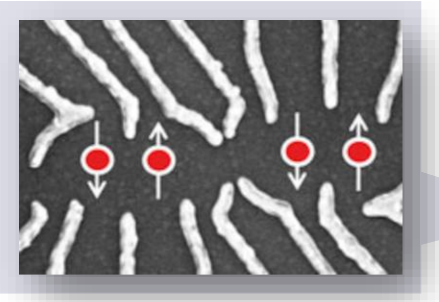
Figure 9 Compilation of carrier mobilities and the corresponding concentration reported values for Cu–Cr–O delafossite. In the brackets are the references from the article. A more detailed survey is presented in supplementary information section—Table S.II.

- Gap: 1.8 eV
- Hole effective mass: 3 m_0



Superconductors oxides

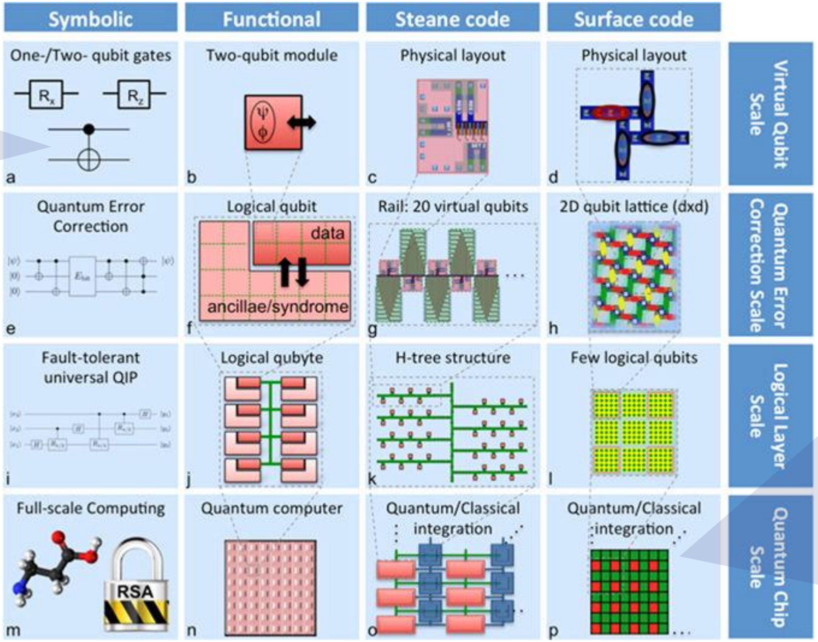
Quantum computing world

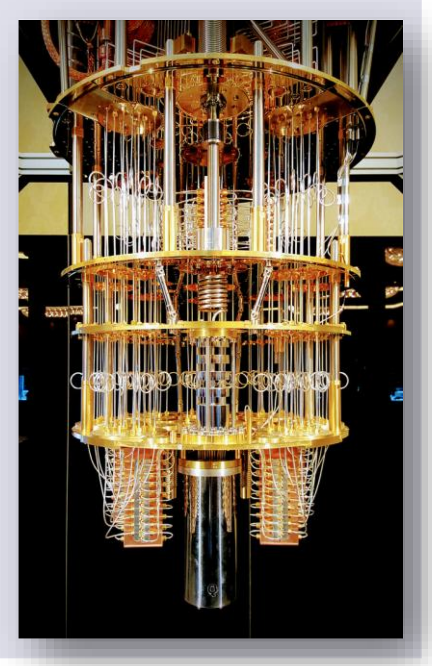


REVIEW ARTICLE OPEN

Quantum information density scaling and qubit operation time constraints of CMOS silicon-based quantum computer architectures

Davide Rotta[1,2,3], Fabio Sebastiano[4], Edoardo Charbon[4] and Enrico Prati[1]

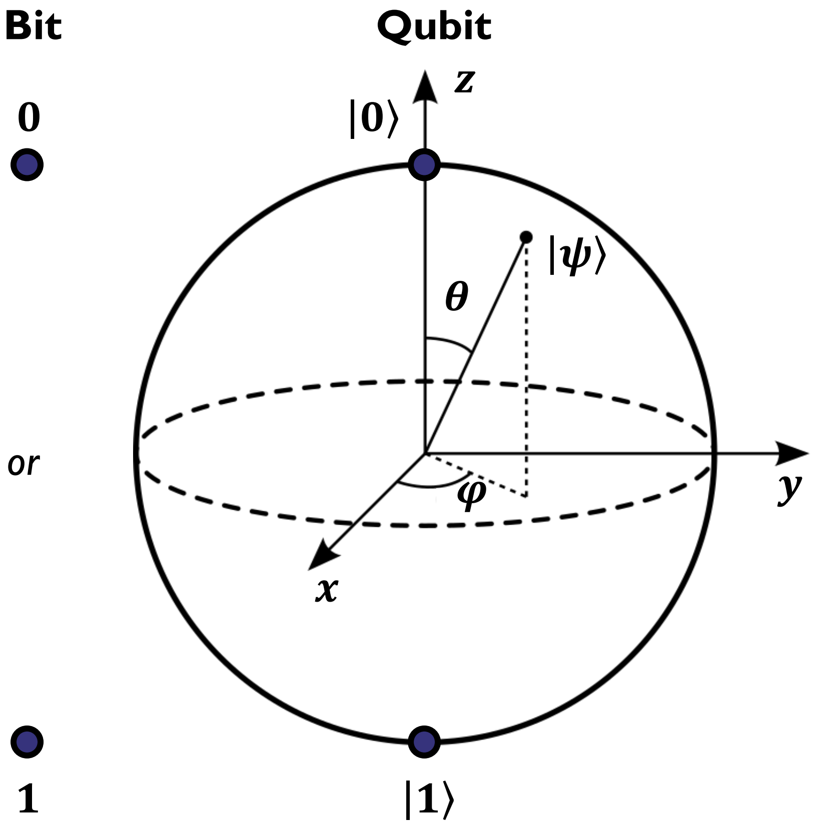




- Qubits are the **building blocks** of quantum computing.

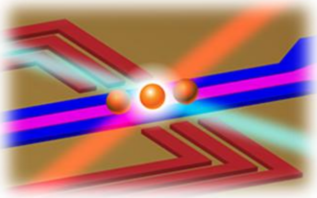
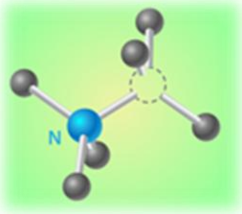
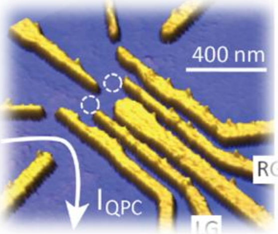
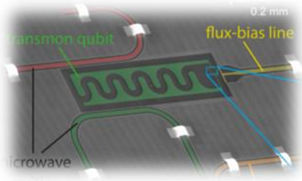
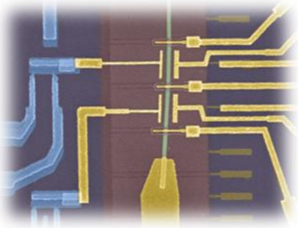
Quantum bit (qubit)

- A **QUBIT**, is the quantum version of a bit.
- Compared to a classical bit, a qubit is a **two-level system** $\{|0\rangle, |1\rangle\}$ that has many more possible states.
- The quantum information stored in a qubit is represented by a linear combination of quantum states with the following wavefunction $|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle$
- The states can be represented by an arrow pointing to a location on the Bloch sphere.



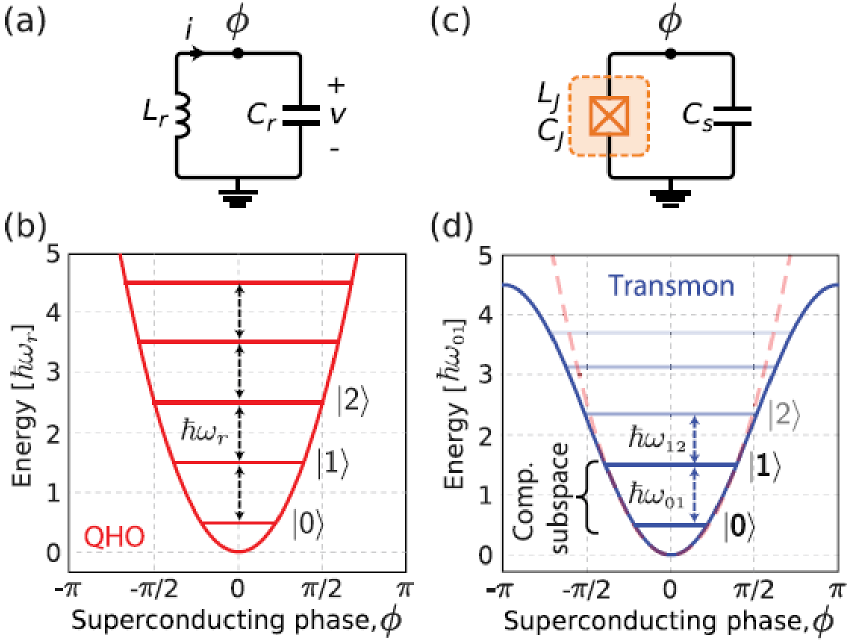
Quantum computing

Qubit technologies

Qubit	Trapped ions	Defects in solids	Semiconductor Quantum Dots	Super-conductors	Topological interfaces
State	Electron	Spin	Spin	Current (phase, charge, flux)	Majorana fermion
Device					
$\|0\rangle$		$\|\downarrow\rangle$	$\|\downarrow\rangle$		|◖⟩
$\|1\rangle$		$\|\uparrow\rangle$	$\|\uparrow\rangle$		|◗⟩

Superconducting qubits

- A Josephson qubit circuit, with a nonlinear inductance $L_j C_j$ shunted by a capacitance C_s is an **anharmonic oscillator**. The Josephson inductance reshapes the quadratic energy potential into sinusoidal, which yields non-equidistant energy levels.
- This allows to isolate the two lowest energy levels $|0\rangle$ and $|1\rangle$, forming a computational subspace with an energy separation $\hbar\omega_{01}$, which is different than $\hbar\omega_{12}$.
- Anharmonicity allows to approximately treat oscillator as a **two-level quantum system**.



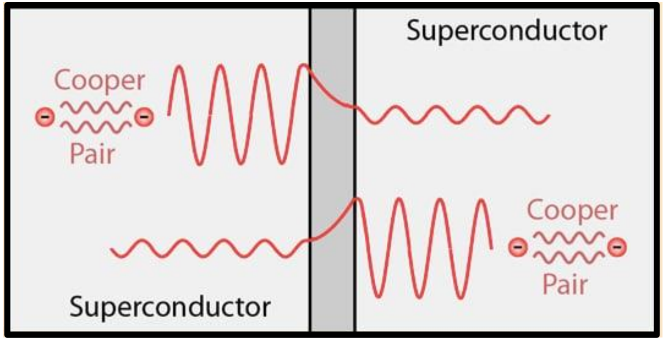
Because the Josephson junction inductance is nonlinear, the qubit potential is anharmonic. The qubit comprises the two-lowest states and is addressed at a unique frequency ω_{01}.

The Josephson junction

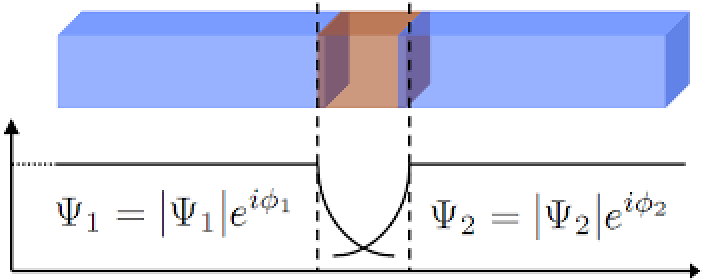
- The Josephson effect produces a current, known as a **supercurrent**, that flows continuously without any voltage applied, across a Josephson junction (JJ).
- Then the *superconducting phase evolution equation* is:

$$\frac{\partial \phi(t)}{\partial t} = \frac{2eV}{\hbar}$$

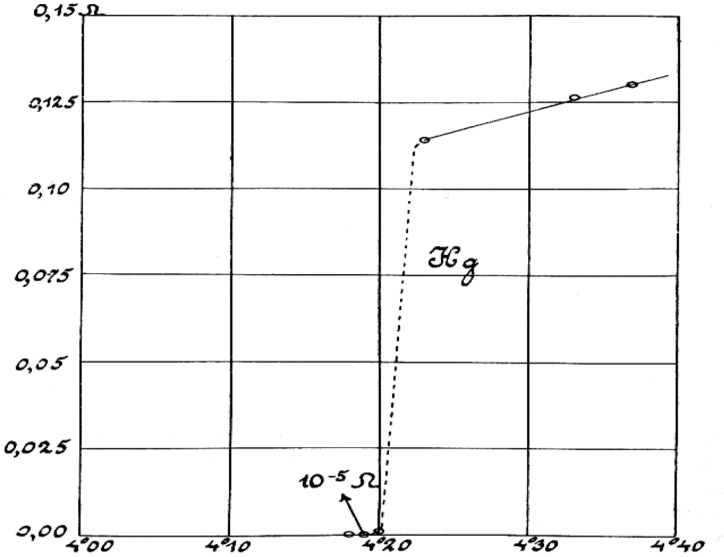
- That is the ratio of change of phase difference is directly proportional to the applied voltage. This means a Josephson junction can act as a **perfect voltage-to-frequency converter**.



Josephson junction



Superconductors

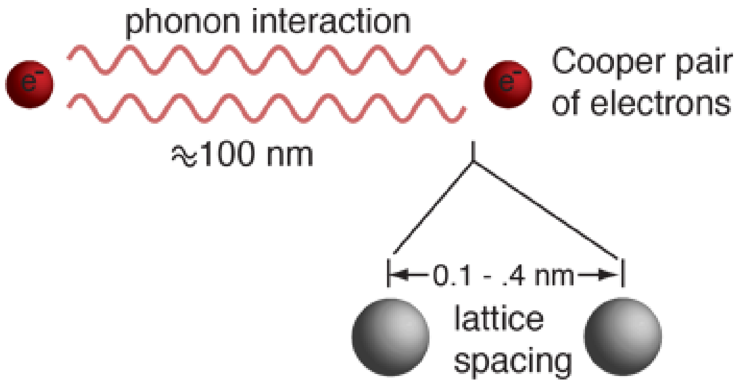


The zero-resistance transition of Hg measured in 1911 by Kamerlingh Onnes.

- Resistivities become zero below a **critical temperature, T_c**.
- The superconducting transition is reversible
- First discovery of superconductivity in mercury Hg in 1911. (H.K. Onnes, Leiden, Holland)

Origin of superconductivity

- Conventional BCS superconductivity (John Bardeen, Leon Cooper, and Robert Schrieffer – Nobel prize 1972) theory is explained by attractive interaction between two electrons of opposite spin through phonons, named Cooper pairs.
- With total spin of 0, Cooper pairs are bosons (no restriction on the occupied energy state)
- In particular, at low temperatures when thermal agitation of atoms is minimal.



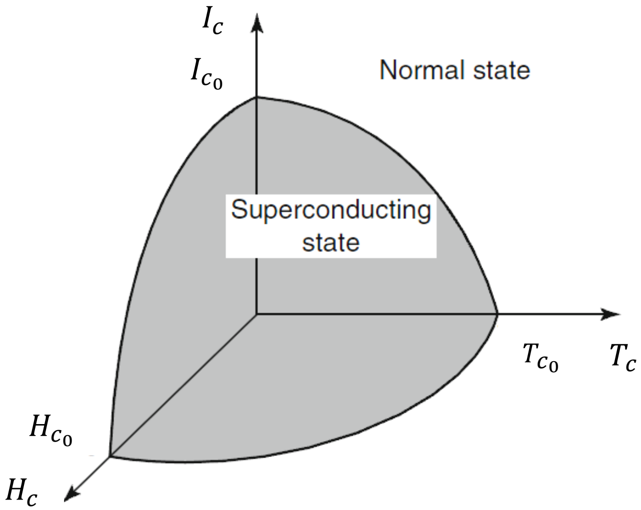
Interaction range of Cooper pairs.

Superconducting state

- “*critical space*”
  - Critical temperature
  - Critical magnetic filed
  - Critical current
- Relationship

$$H_c = H_{c_0}\left(1 - \frac{T^2}{{T_c}^2}\right)$$

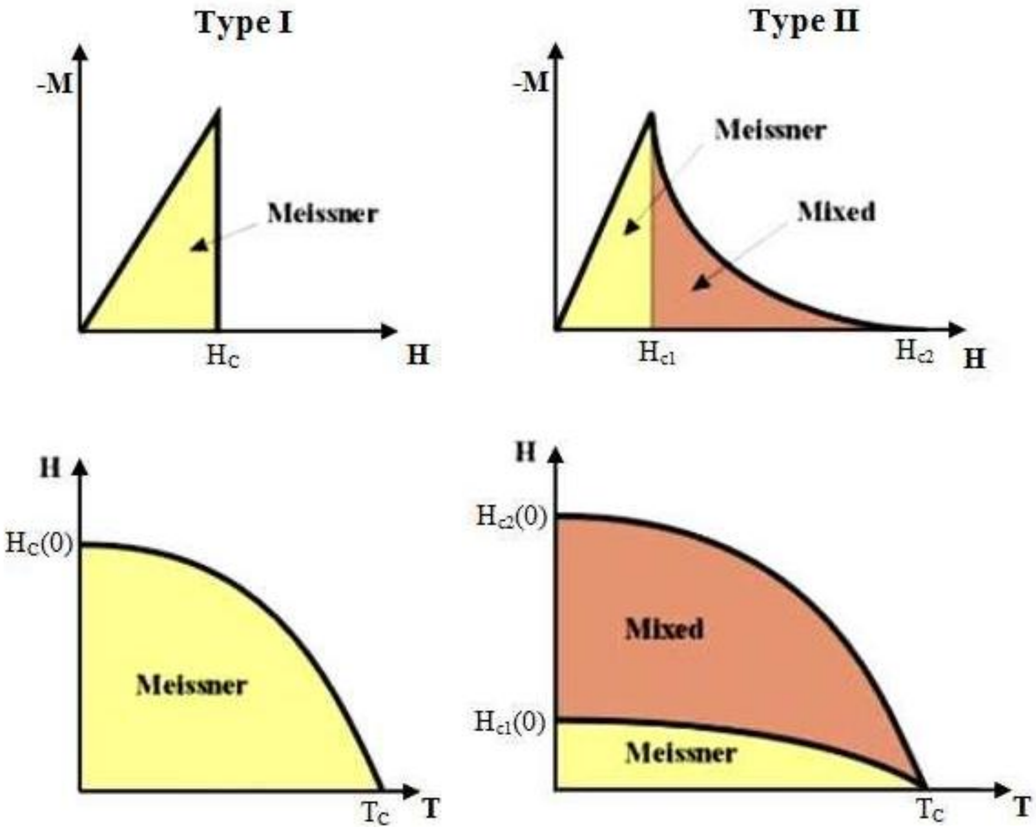
- An increase in one of these parameters decreases the critical value of the remaining two.



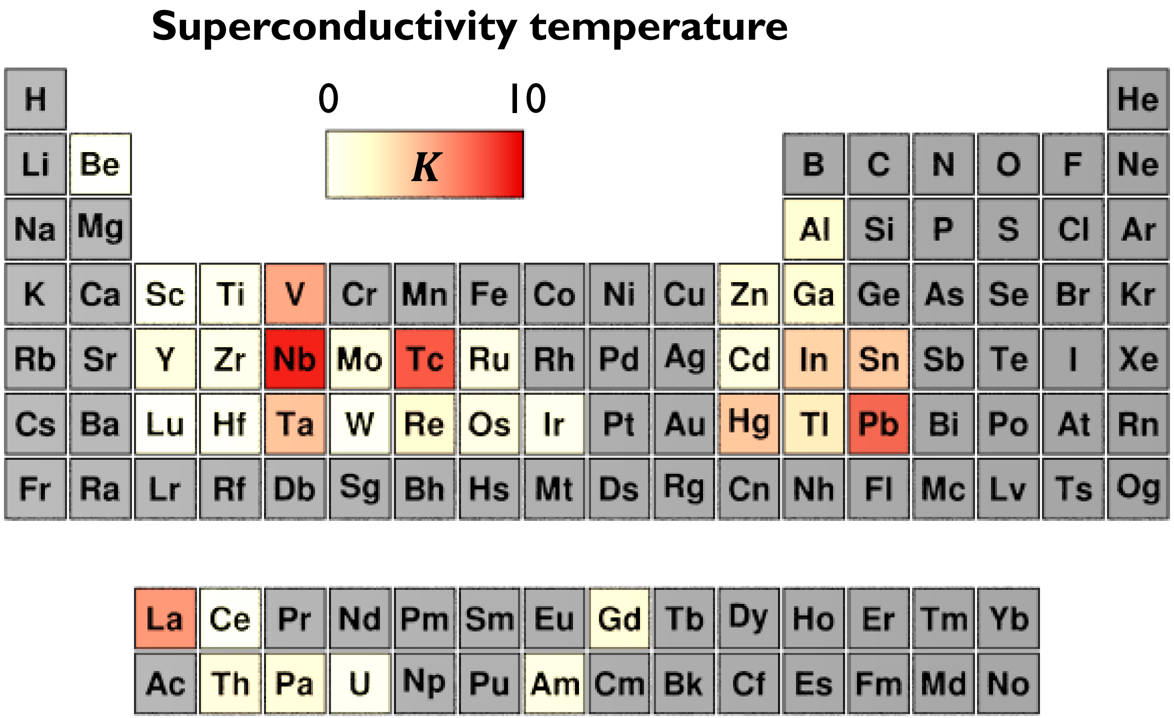
The limits of superconductivity are defined in a critical T-H-I-diagram.

Type I vs Type II superconductors

- Type-I superconductors are superconducting materials that **lose their superconductivity very easily or abruptly** when placed in an external magnetic field.
- Type-II superconductors are superconducting materials that **lose their superconductivity gradually** when placed in the external magnetic field.
- In type-II superconductor, T_c, H_c and J_c values are very large comparison with type-I superconductor.



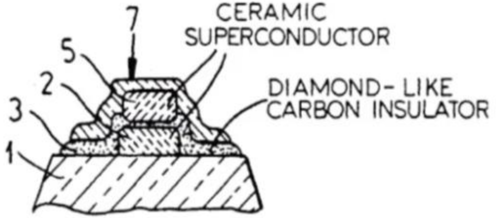
Superconductor materials



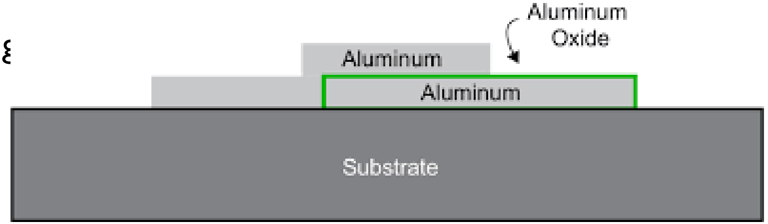
- While most elemental superconductors belong to the type-I category
- Niobium (Nb), Vanadium (V), and Technetium (Th) are elemental type-II superconductors

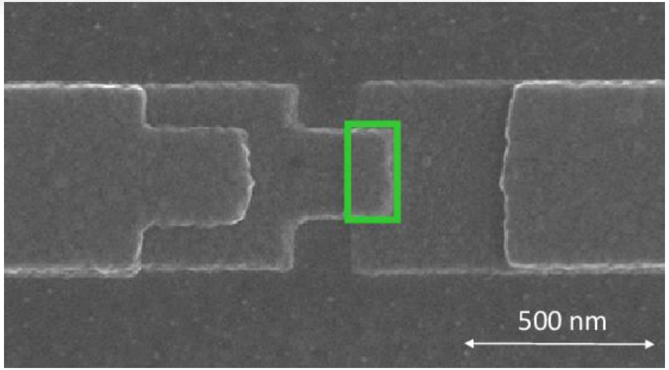
Josephson junction fabrication

- Superconductor
- Patterning
- Insulating layer
  - Oxide: Al_2O_3, MgO, …
  - Non-oxide: CaF_2, MgF_2, diamond-like carbon
- (Patterning)
- Superconductor
- Patterning
- Final sealing and coating



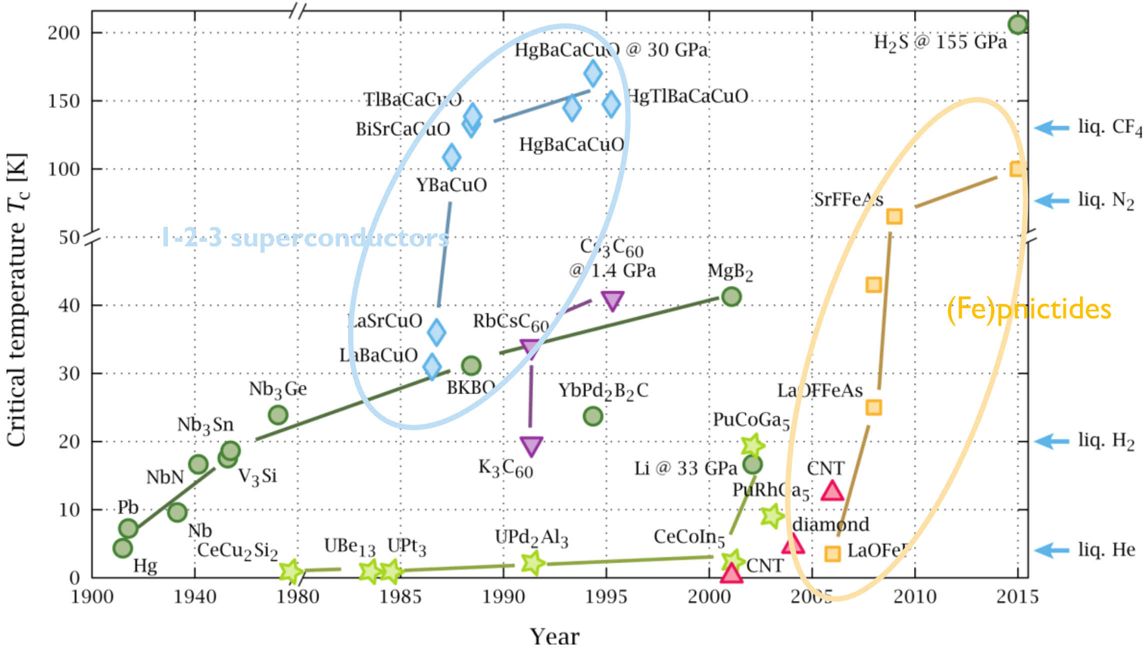
Reference- Aharon Z. Hed, "Method of Making a Josephson Junction", U.S. Patent, 5171732, Dec 15,1992.





Superconductors materials

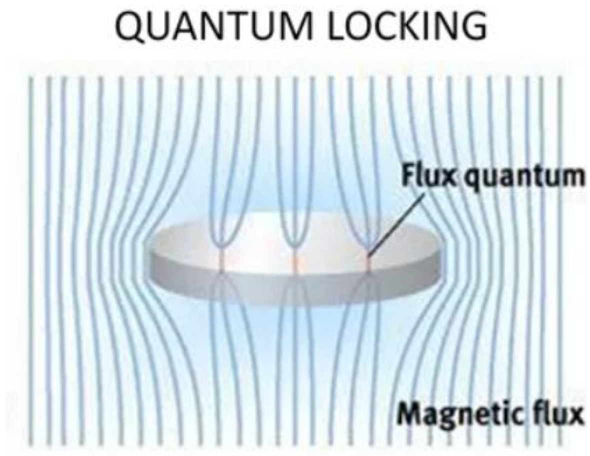
- In 1986, a new class of superconductors was found by Bednorz and Müller (IBM Zurich, Switzerland) which involved copper oxide-based ceramics.
- Type-II superconductors include YBCO (Yttrium-Barium-Copper-Oxide), which is famous as the first material to achieve superconductivity above the boiling point of liquid nitrogen (77 K).

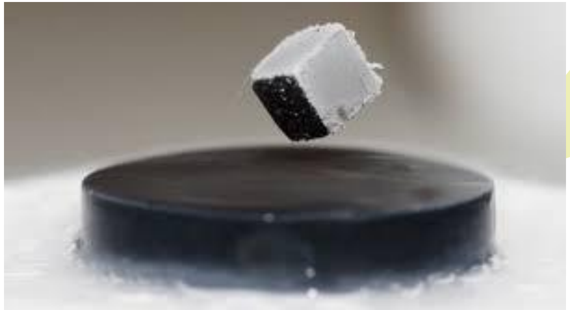


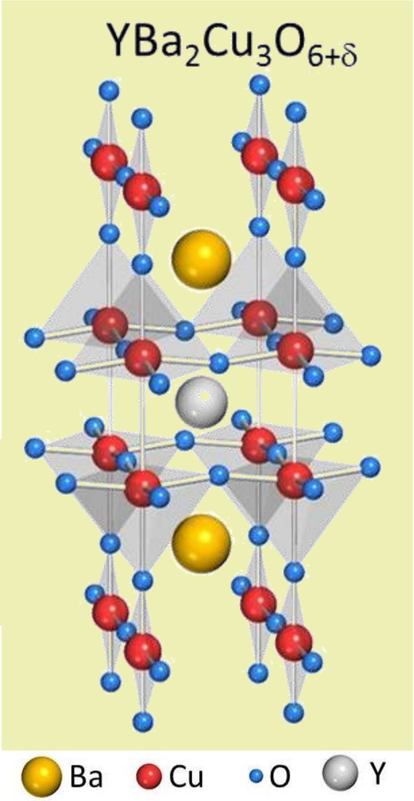
Overview of superconducting critical temperatures for a variety of superconducting materials since the first discovery in 1911.

Quantum levitation

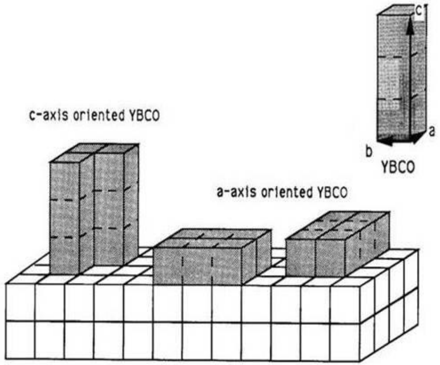
- Type-II superconductor made of ceramic compound $YBa_2Cu_3O_{6+\delta}$, with T_c = 93 K.
- Quantum locking effect
- Type-II based superconducting currents develop vortices pinning the magnetic flux within the materials and levitating the magnet above the YBCO crystal …

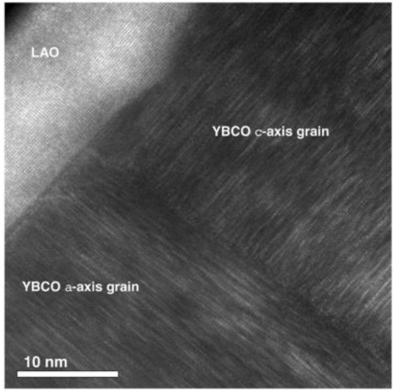






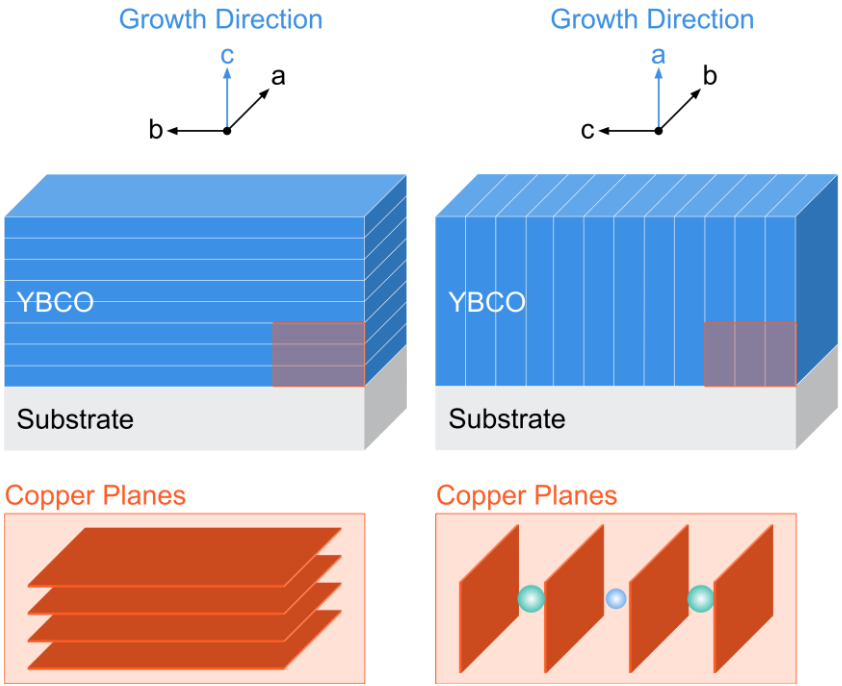
YBCO materials





Supercond. Sci. Technol. 17 (2004) 1–6

- c-axis epitaxial growth.
  - CuO_2 planes in sheets orientation
- a-axis epitaxial growth.
  - CuO_2 planes in walls morphology



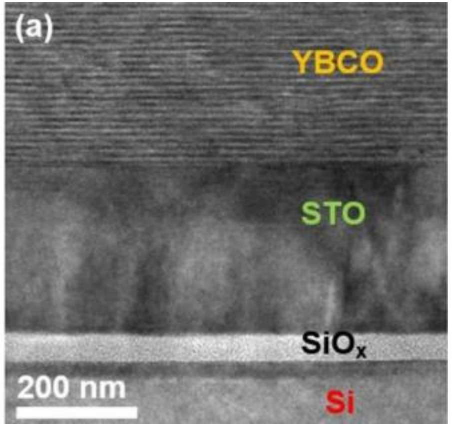
www.ambature.com

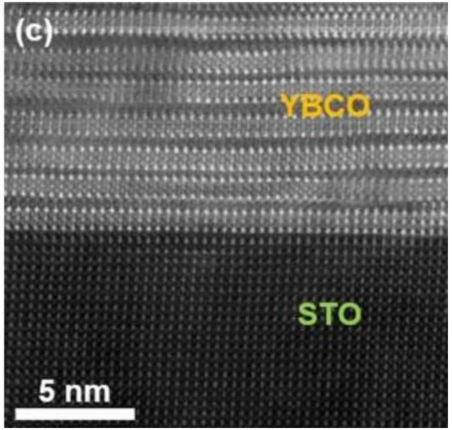
c-YBCO on Si(001)

Bull. Mater. Sci. (2018) 41:23

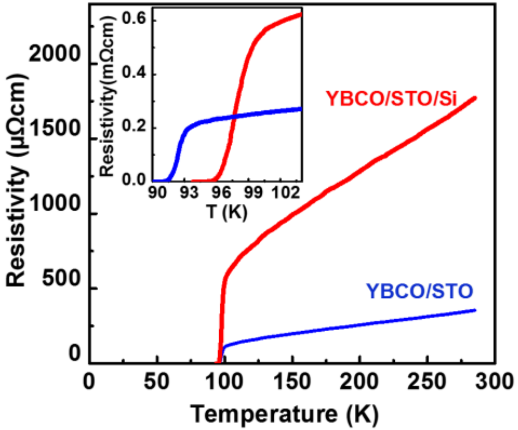
Using PLD, grown at 860 ^{0}C

Using MBE, grown at 650 ^{0}C

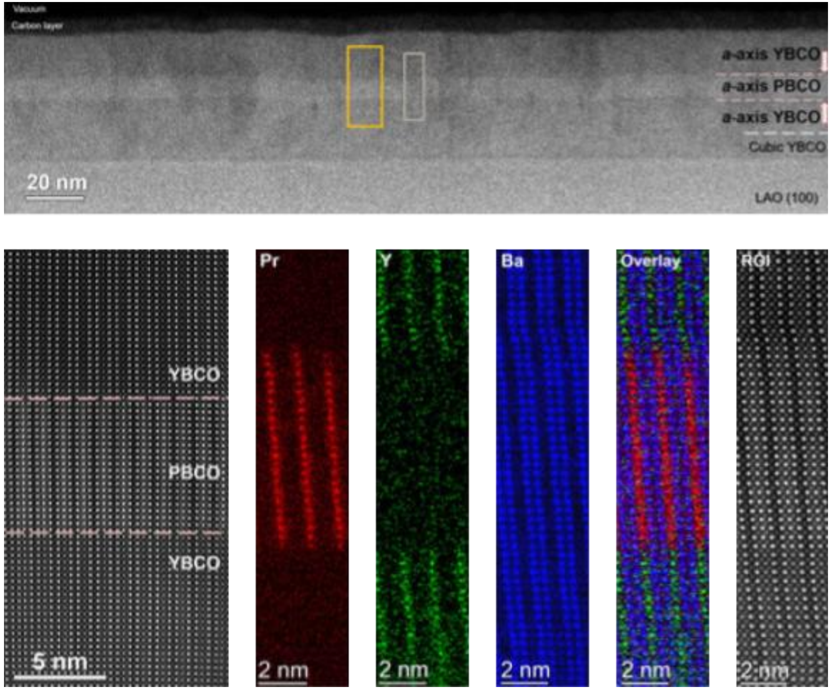




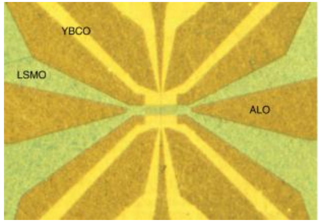
- YBCO SC grown by PLD on STO/Si
- High crystalline quality on Si, but higher resistance compared to YBCO on STO(001) bulk.
- High-T_c > 90 K

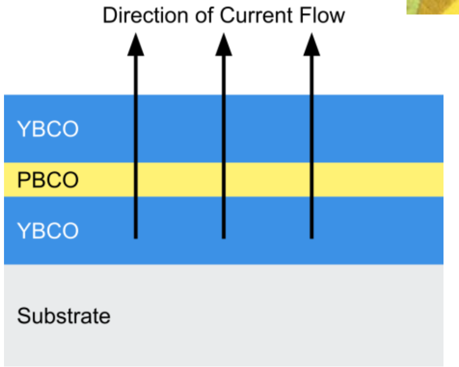


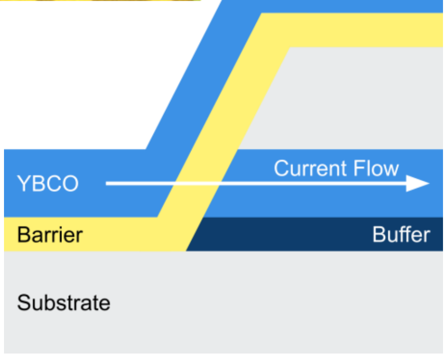
YBCO-based Josephson junction



APL Mater. 9, 021117 (2021)

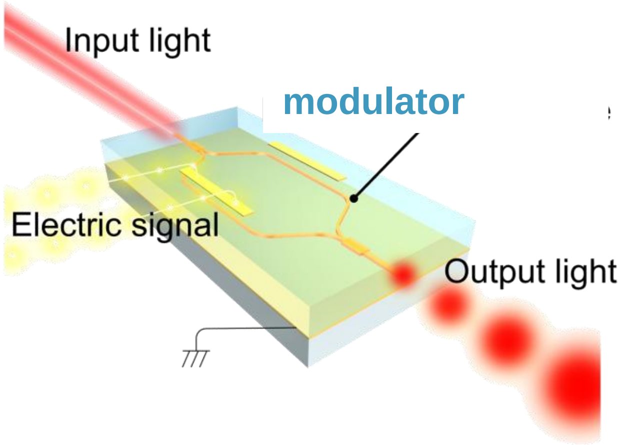






- Epitaxial YBCO-based JJs
- Different device design strategy for a-axis vs. c-axis epitaxial JJs
- First demonstrations with T_c > 100K !

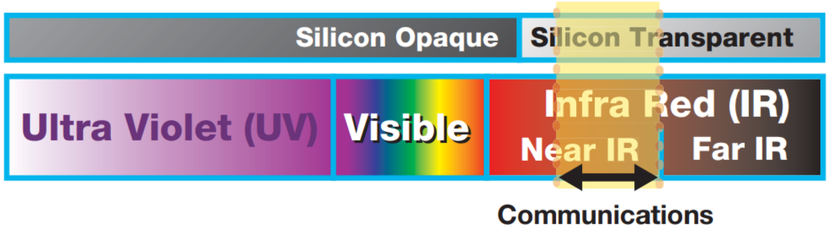
Electro-Optical oxides

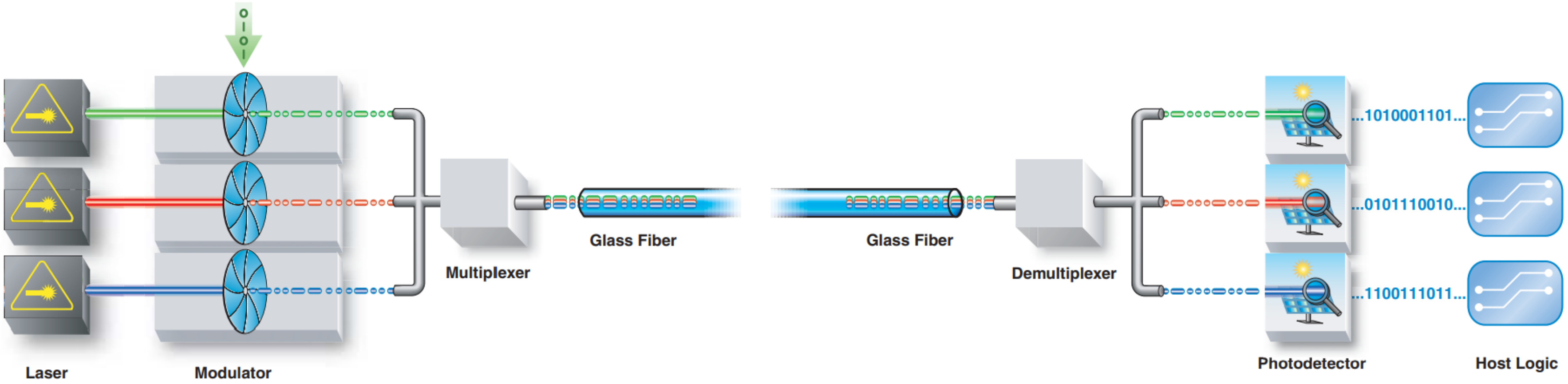


Photonic Integrated Circuit (PIC)

Introduction

- Use of light to transmit data (farther and faster than copper)
- Basic transmitter & key components

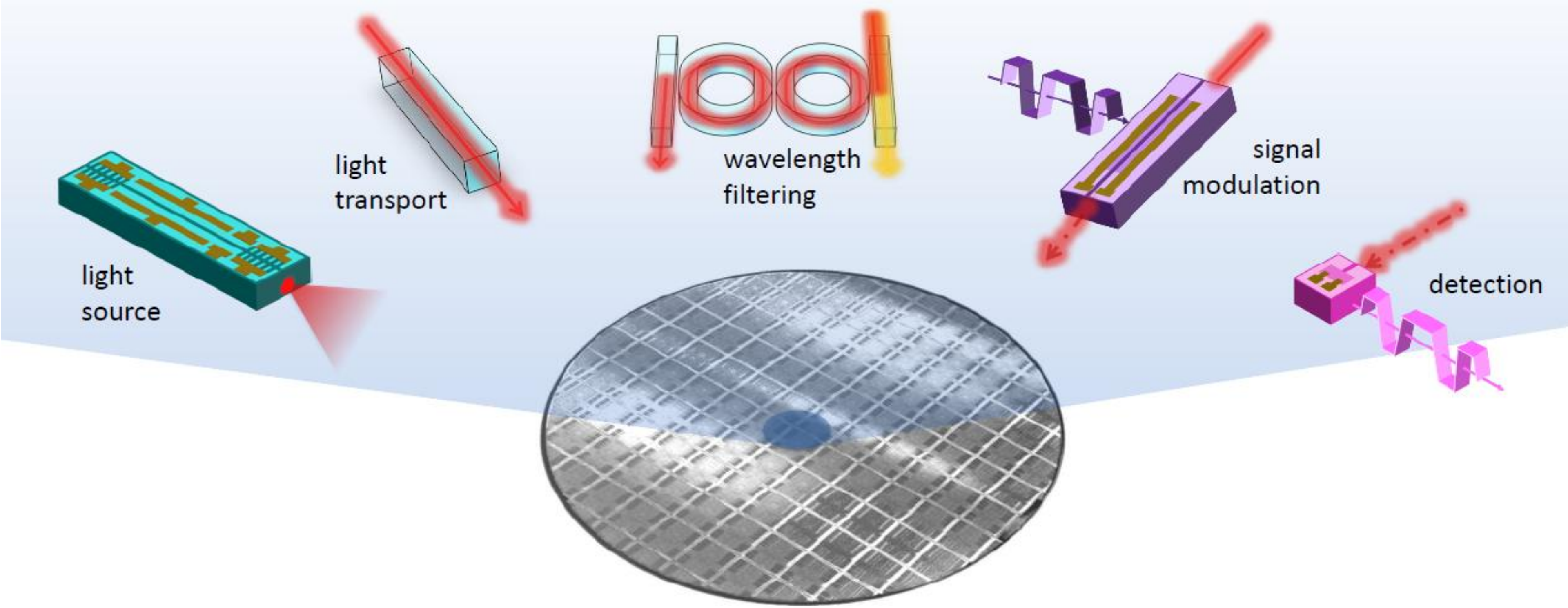




Courtesy of Wim Bogaerts – Univ. Ghent & imec (2020)

Photonic Integrated Circuit (PIC)

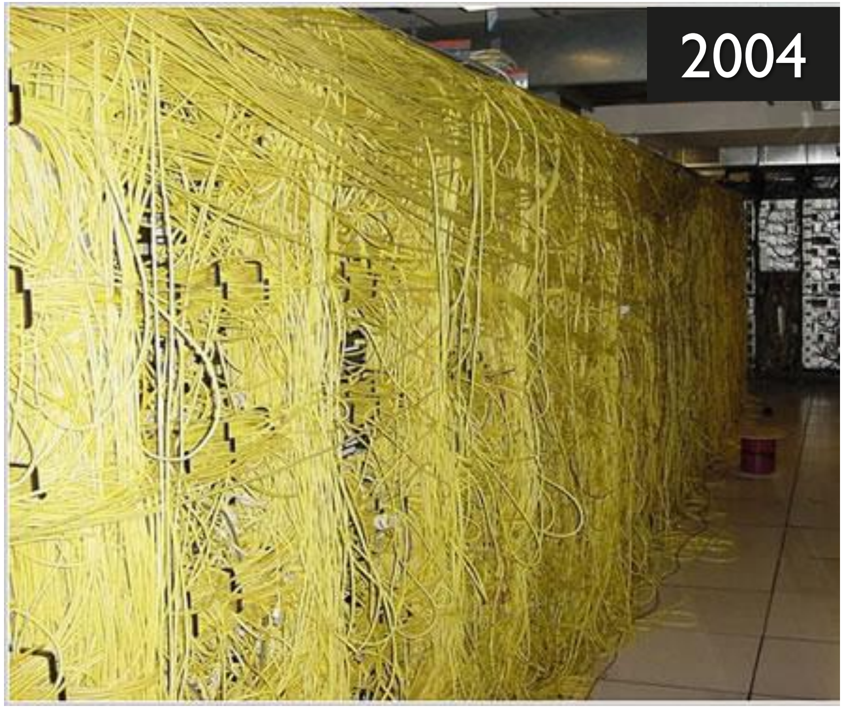
Basic components



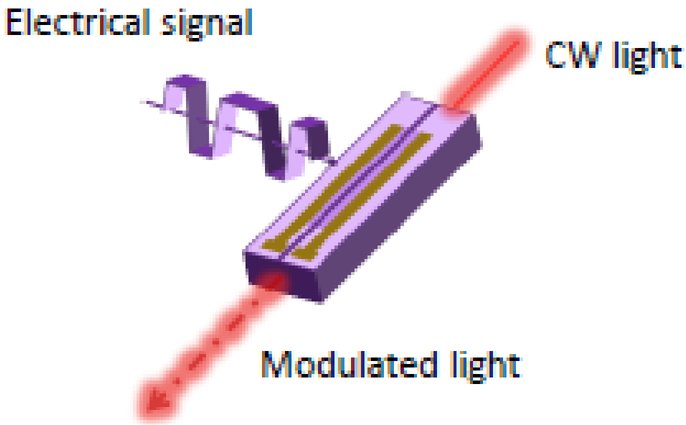
Courtesy of Christian Haffner - imec (2025)

Data centre evolutions

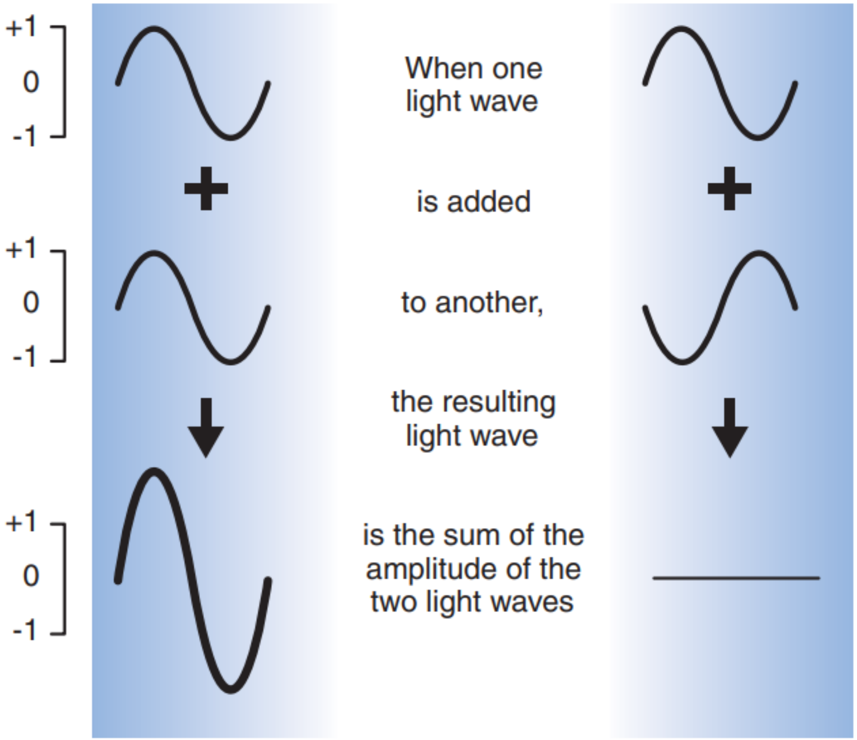
From electrical cables to optical fibres



Modulators



- Laser ON/OFF is not efficient…
- Phase shifting will encode the data by changing the brightness of the lightwave.



When one light wave

is added

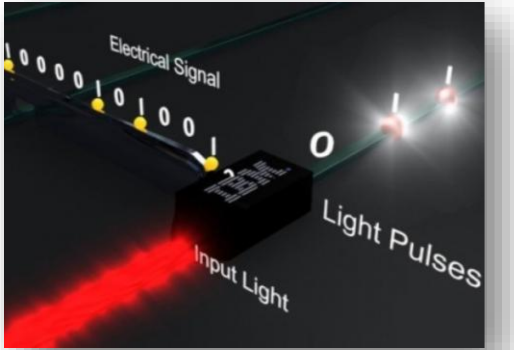
to another,

the resulting light wave

is the sum of the amplitude of the two light waves

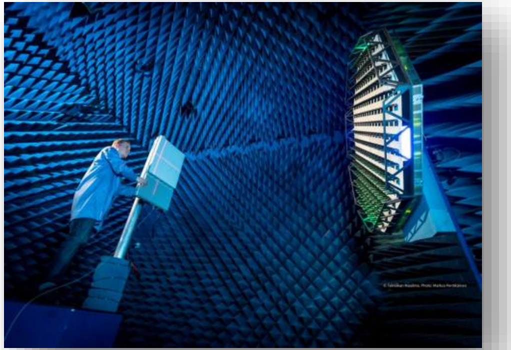
Intel (2010)

Wide Range of Potential Applications



Optical modulators

Video holography



Beamforming

Quantum communication

AR/VR

Automotive

Modulator technology landscape

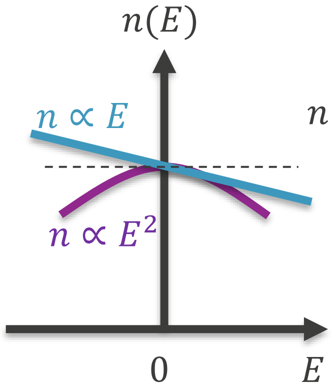
Phase shifter	$V_\pi L$	Optical losses	Operation frequency	Power consumption	Integration process
Depletion p/n	*Fair*	*High*	*50 GHz*	*fair*	*FEOL*
Thermo-Optic	*Low*	*Low*	*100's kHz*	*High*	*BEOL*
$LiNbO_3$ (LNO)	*Large*	*Low*	*100 GHz*	*Low*	*Far BEOL*
MEMS	*Very Low*	*Low*	*MHz*	*Low*	*F/MEOL*
$BaTiO_3$ (BTO)	*Low*	*Low*	*???*	*Low*	*F/MEOL*
EO polymer	*Low*	*High*	*> 100 GHz*	*TBD*	*Far BEOL*

BTO is the only material that ticks all the boxes

- Electro-optical material
- Compatible with CMOS infrastructures
- To enable the system most compact, low loss & high-speed

Electro-Optical Fundamentals

- E-O effect is the change of refractive optical index (n) of a material induced by an external electric field, ideal for light modulation...
- Refractive index



$$n(E) \approx n \underbrace{- \frac{1}{2} r n^3 E}_{\text{Pockels effect}} \underbrace{- \frac{1}{2} \xi n^3 E^2}_{\text{Kerr effect}}$$

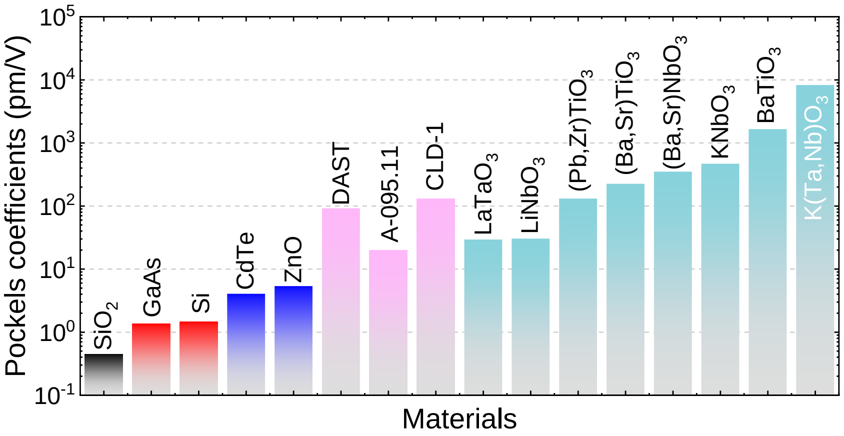
- Pockels coefficient

$$r_{ijk} = \varepsilon_0 f_{ijm} (\varepsilon_{mk} - \delta_{mk})$$

Polarization-optic coef.

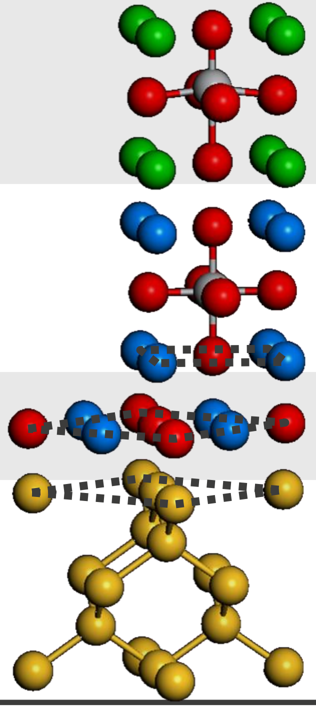
Dielectric constant

Dielectric loss



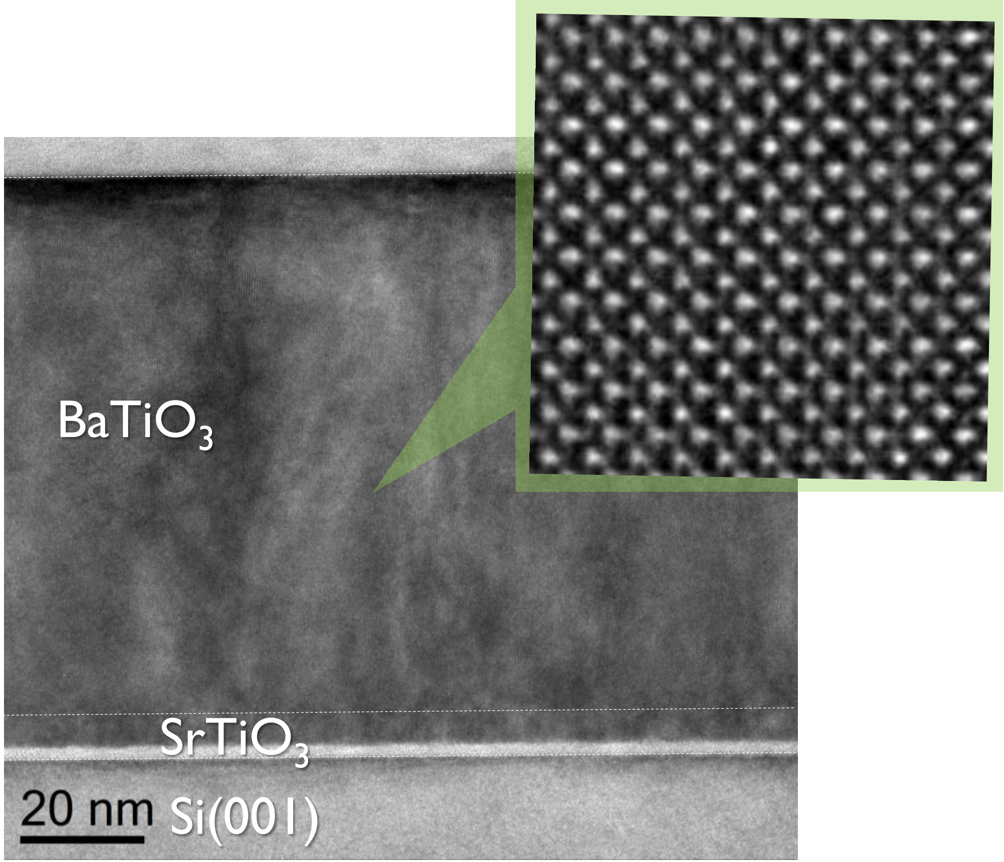
- Large electro-optic effects would be observed in materials with:
  - large polarization-optic response
    - Organic polymers & organic crystals
  - large dielectric constant
    - Ferroelectric oxides (BTO, KNO, ...)
- Applications / devices
  - Photonic, beam forming, quantum, display, …

$BaTiO_3$ on Si(001)



	Material
Active	$BaTiO_3$ *Perovskite*
Buffer	$SrTiO_3$ *Perovskite*
Interface	**½ ML SrO** *Rocksalt*
Substrate	**Si(001)** *Diamond*

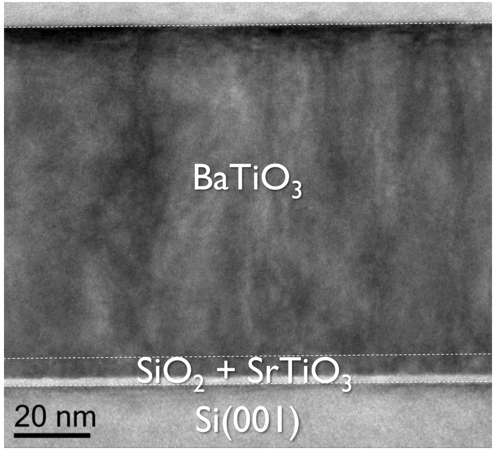
[100]ABO_3(001) // [110]Si(001)



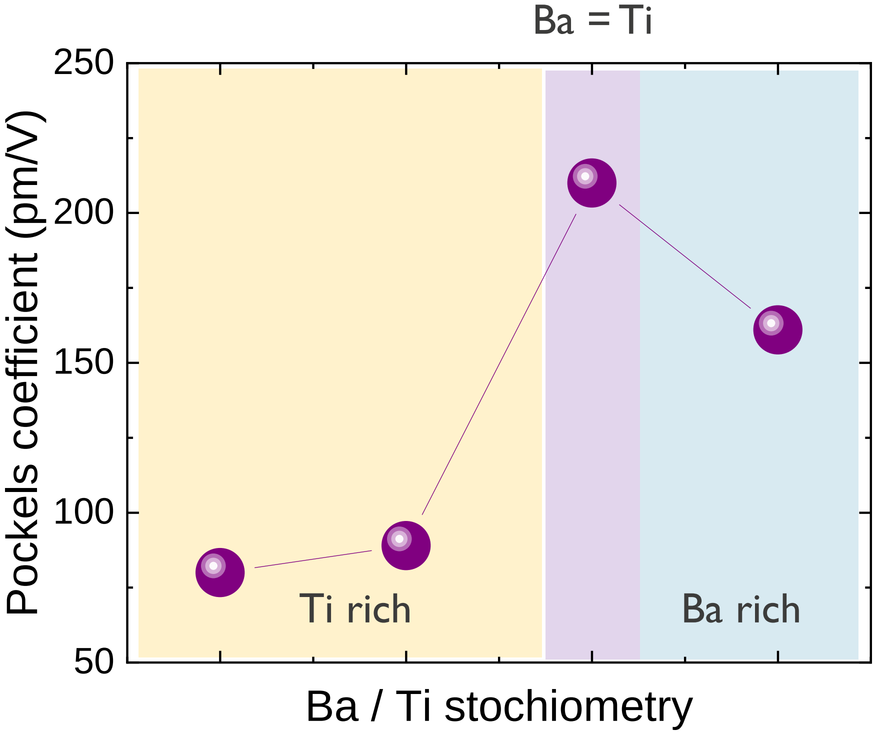
[1] M. Hsu et al, Appl. Phys. Express (2017), [2] C. Merckling et al., JVSTA (2019)
[3] TH Wang et al., Journal of Crystal Growth, (2022), [4] M. Baryschnikova et al., Crystals (2024)

$BaTiO_3$ on Si(001) heterostructures

Solid-source MBE approach



- High $BaTiO_3$ quality obtained by SS-MBE
  - Monocrystalline heterostructure & atomically smooth surfaces
  - Pockels coefficient is highly stoichiometry dependent !

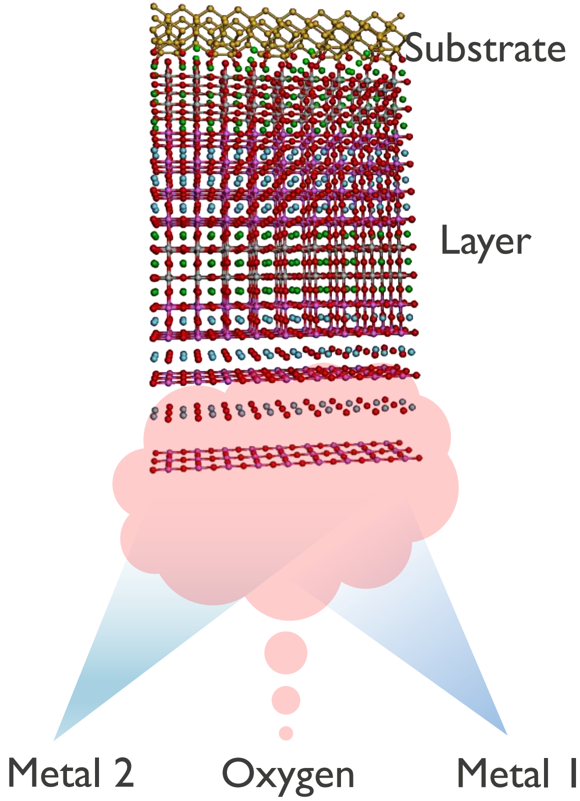


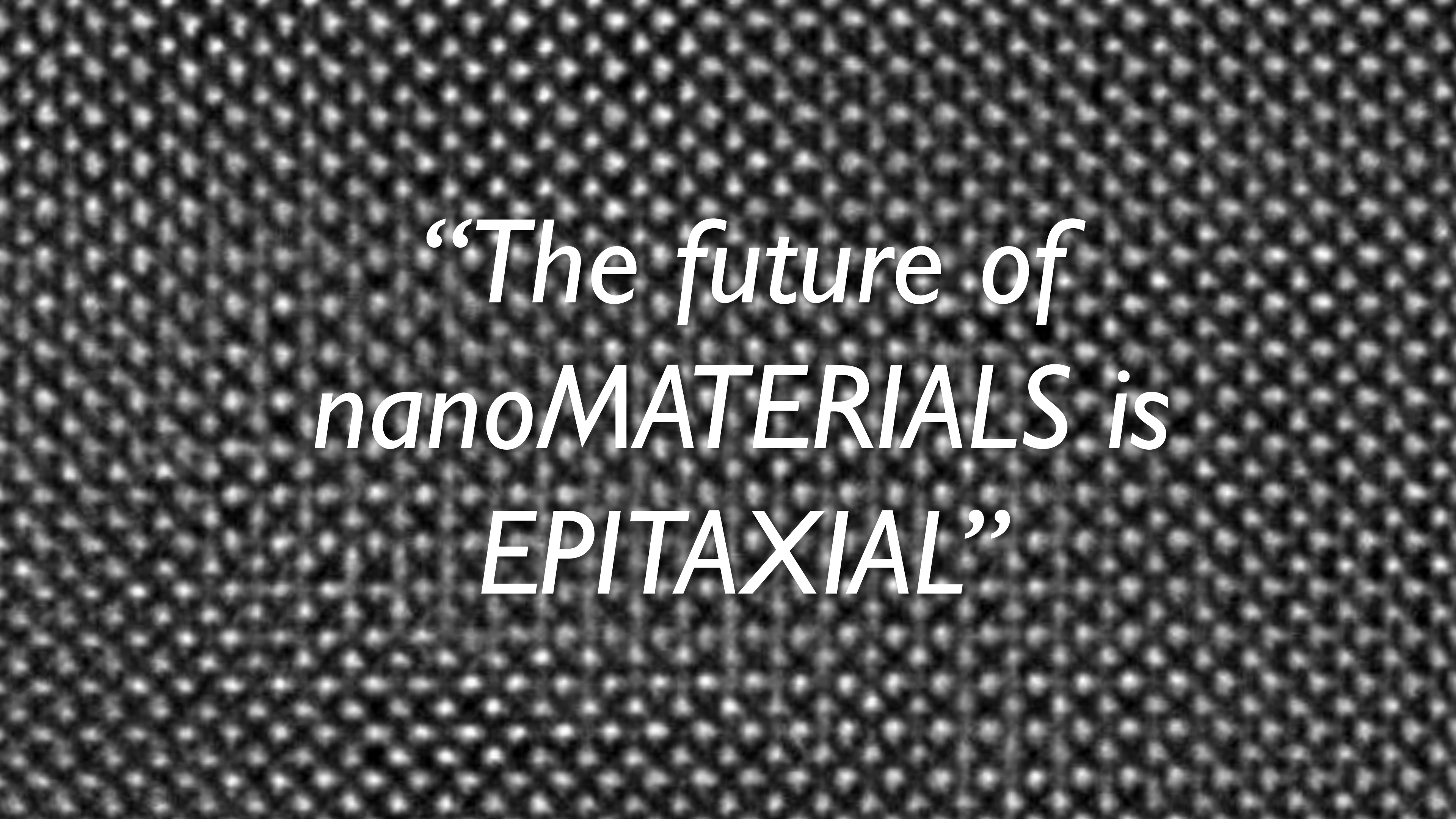
Conclusions

Wrap up

Conclusions

- Future device trends: scaling continues, new materials needed
- Metal-oxides open new and unique functionalities
- Complex (perovskite) heterostructure with coherent interfaces for exploratory devices (logic, memory, quantum, photonic ...)





“The future of nanoMATERIALS is EPITAXIAL”

Acknowledgements

- Alumini
    - Dr. W. Mortelmans (intel), Dr. M. Hsu (Apple), Dr. T. Wang (TSMC), Dr. S. Hasan (Aixtron), Dr. S. El-Kazzi (Aixtron), Dr. S. Jiang (GF), Dr. Z. Liu (Huawei)
- KUL/imec PhDs
    - I. Ahmed, L. Ceccon, A. Boelen, B. Pollefliet, A. Ulrich, M. Rohde (+UCL), K. Brahim, A. Varanasi, A. Aparna, Y. Ozdemir, H. Tran, Y. Yang, H.-Y. Lee, H. Dongre, M. Gambin, H. Cuma
- imec scientists
    - Dr. M. Baryshnikova, Dr. G. Croes, Dr. C. Haffner, Dr. G. He, Dr. S. Sutar, Dr. K. Banerjee, Dr. C. Porret, Dr. J. Donohue, Dr. S. Sharif Azadeh, Dr. M. Kaviani, Dr. H. Sharma
- imec HW & ENG team
    - H. Costermans & K. Dubois
- imec management
    - Dr. J. Swerts, Dr. F. Holsteyns, Prof. S. De Gendt, Dr. P. Soussan, Dr. C. Lockhart de la Rosa, Dr. G. Sankar Kar, Dr. S. Scheer
- Sponsors & fundings
    - imec core partners
    - ERC (NOTICE ga. 864483, Q-Amp ga. 101042414)
    - EOS CONNECT (FWO/FNRS)
- Collaborators
    - VEECO: Dr. S. Farrell, Dr. M. O'Steen, Dr. R. Metha, Dr. G. Sundaram
    - KUL: Prof. F. Molina Lopez, Prof. J. van de Vondel, Prof. L. Peirrera
    - UCL: Prof. P. Gehring
    - PSI: Dr. M. El-Kazzi

European Research Council

"This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 864483)".

Thank you !

Any questions ?