



1.7 nm

Nanostrukturierte Beschichtungen:

Wenn die Architektur wichtiger wird als die Chemie

swiss mnt network: "Trends in Mikro-Nano"

Hochschule Luzern Technik & Architektur

Donnerstag, 5. Dezember 2013

Dr. Pierangelo Gröning (pierangelo.groening@empa.ch)

Head of the Department "Advanced Materials and Surfaces"

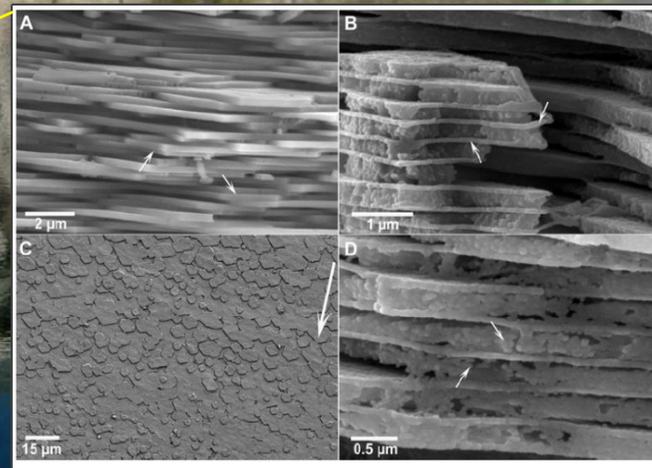
Ueberlandstrasse 129

CH-8600 Duebendorf

Function follows Architecture



Inspired by Nature



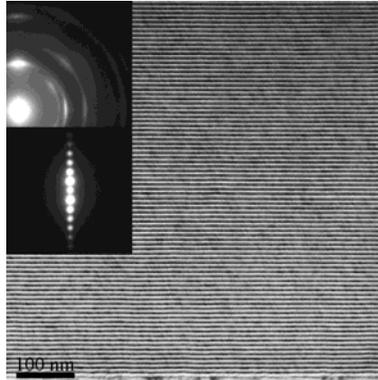
Photos: Fabio Nudelman, Weizmann Institute

... novel materials and coatings with well defined architectures on the nano-scale.

Nanostructured Thin Films and Coatings

Hardening via Interfaces

TiN/SiN_x Multilayer Coating



Hardness TiN: ~ 30 GPa

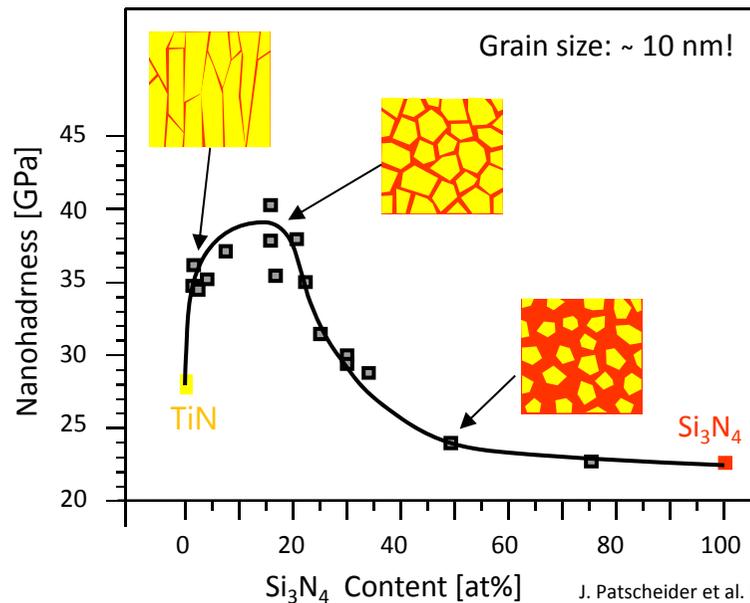
Hardness : ~ 50 GPa

$d_{\text{TiN}} = 4.5 \text{ nm}$ (dark)

$d_{\text{SiN}_x} = 2.8 \text{ nm}$ (bright)

University of LULEÅ (S)

Superhard n-c:TiN/Si₃N₄ Coatings



Ti⁰, Si⁰, N₂, Ar

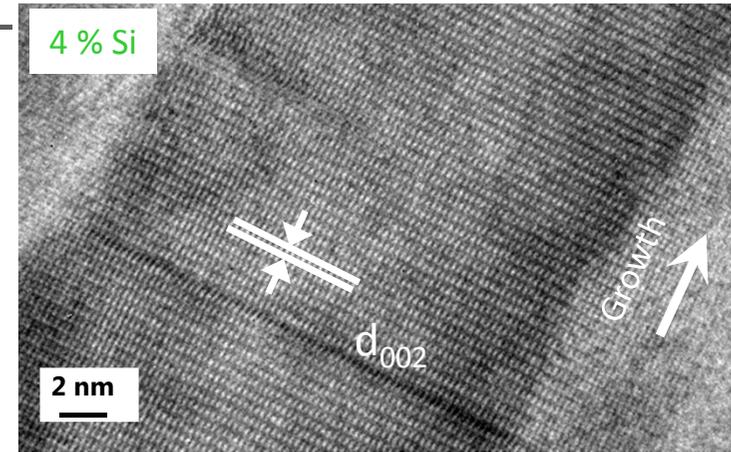
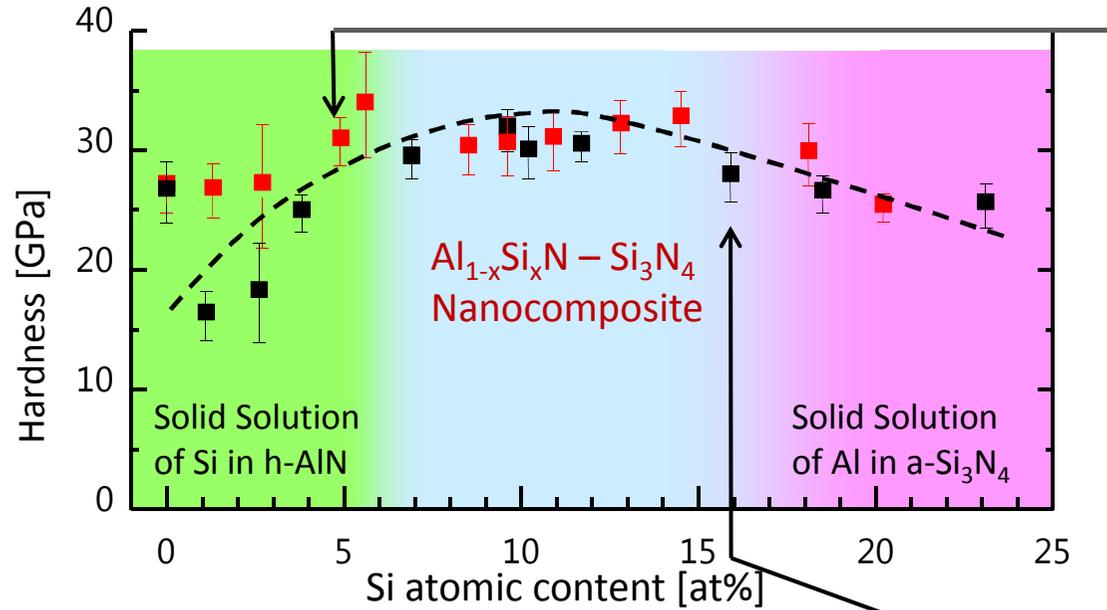
T_{dep.} = 200 – 350°C

U_{bias} = - (70 – 120V)



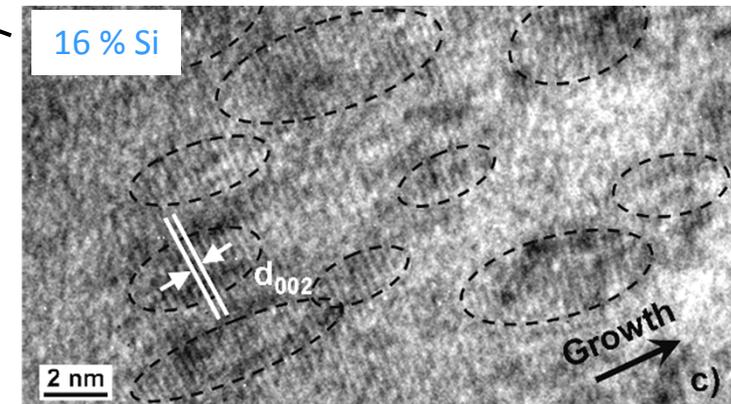
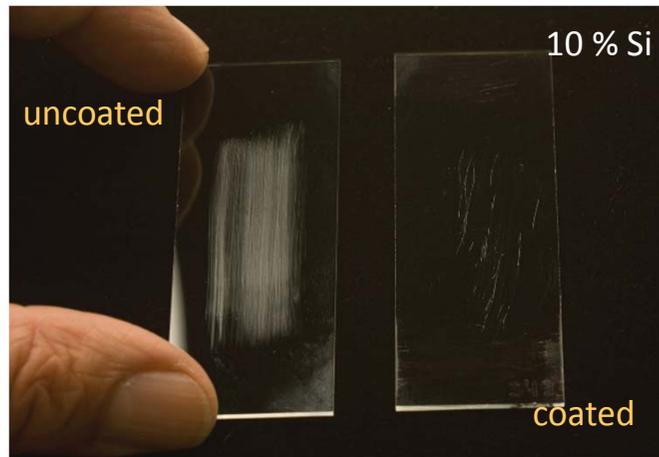
Nanostructured Thin Films and Coatings

Transparent Hard Coating: $Al_{1-x}Si_xN - Si_3N_4$

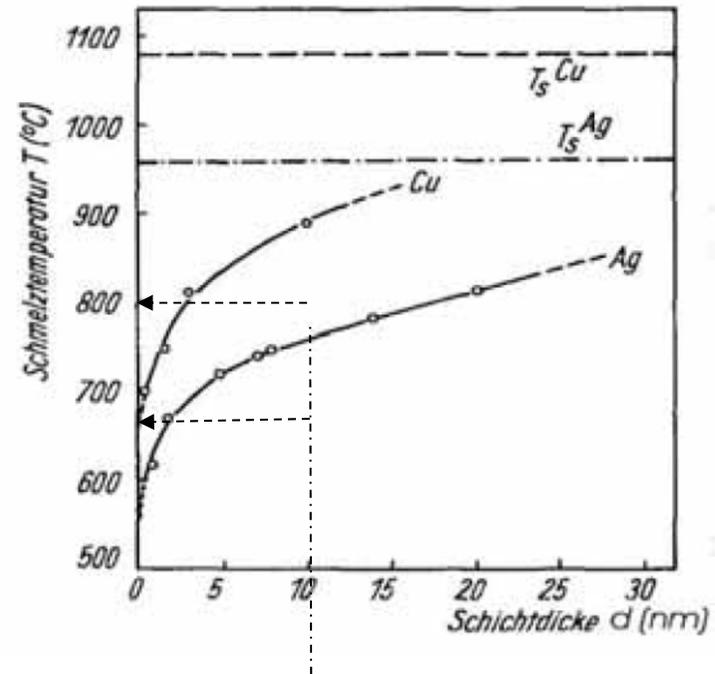
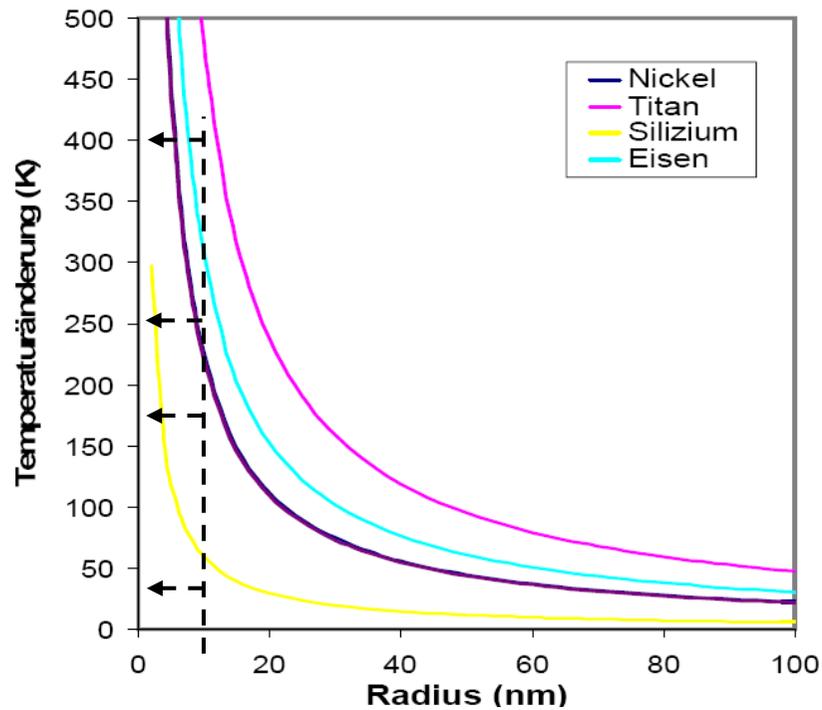


HRTEM of $Al_{1-x}Si_xN$ crystallites in Al-Si-N

Scratching with SiC paper



Joining: Melting Point Depression



$$\Delta T = (T_s - T) = \frac{2\sigma \cdot T_s}{\rho \cdot L \cdot r} \sim \frac{1}{r}$$

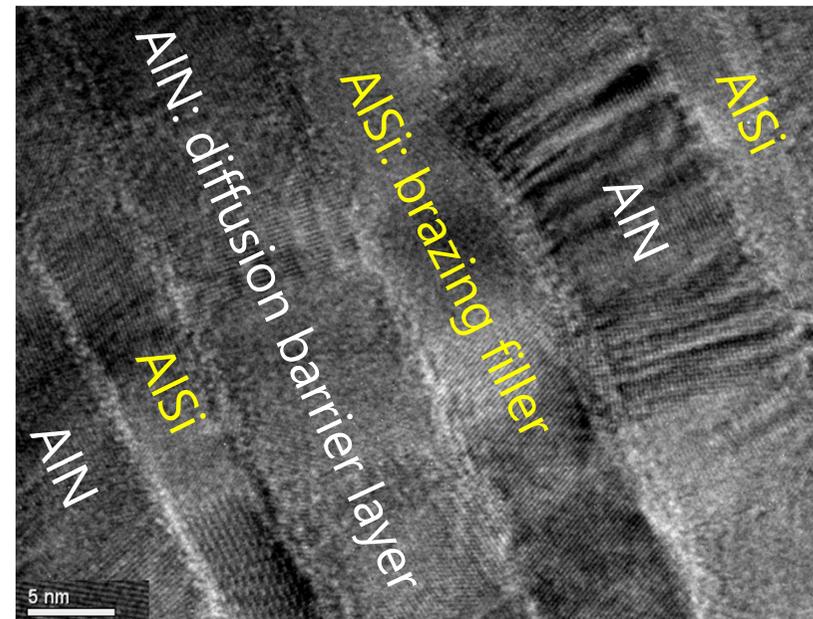
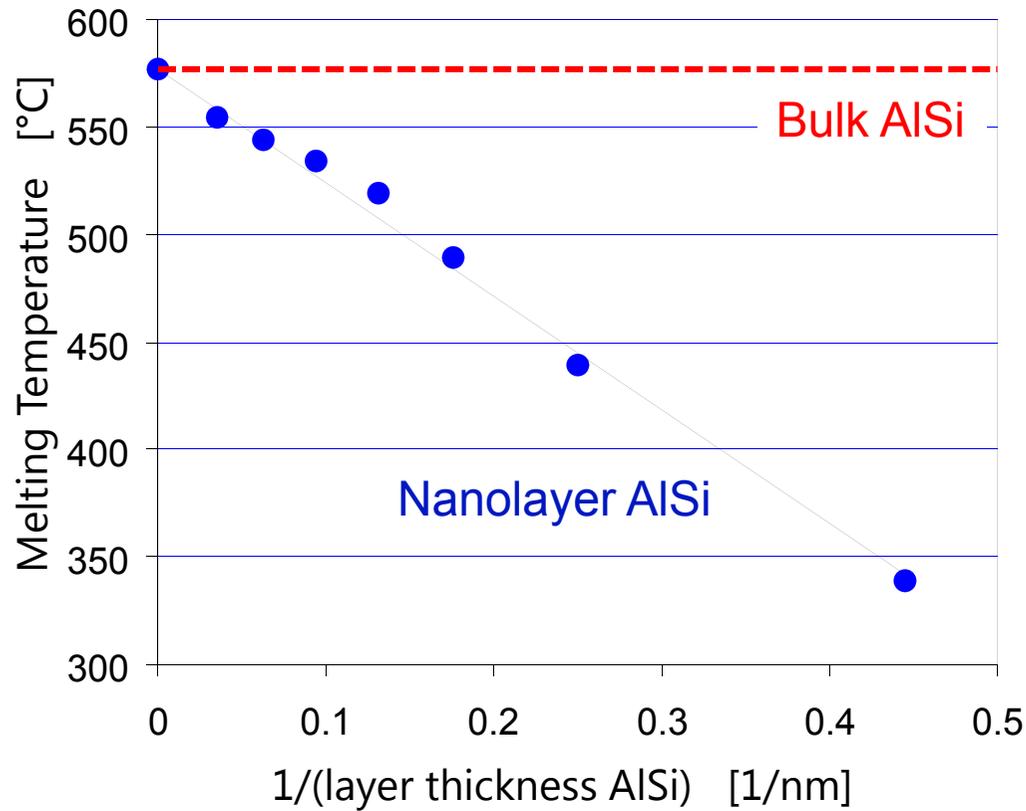
$$T_s(d) = T_s \cdot e^{-\frac{\sigma v}{Ld}}$$

- T_s : bulk melting temperature
- σ : solid-liquid interface energy
- L : bulk heat of fusion
- ρ : density of particles
- r : particle radius

Discovered in 1954 by M. Takagi
Source: Wilden, DVS Forschungsseminar, 2006

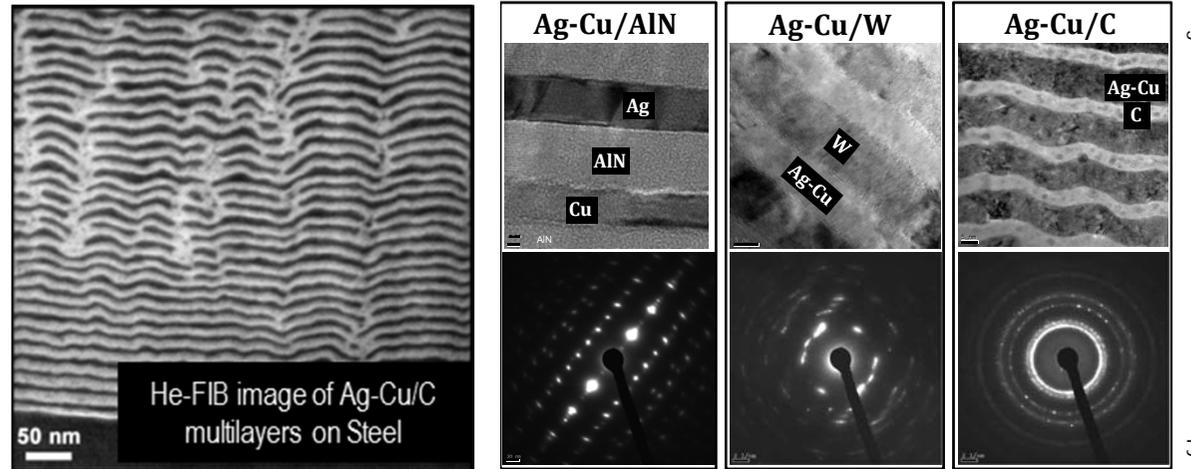
Nano-Brazing Fillers for Joining of Al-Alloys

Melting temperature of AlSi in AlN/AlSi nano-multilayers



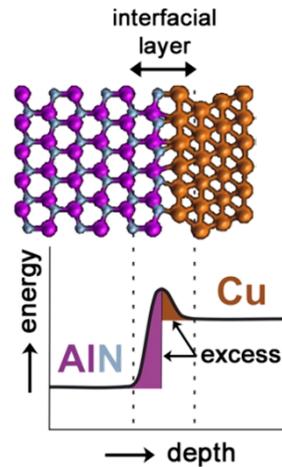
Nano-Brazing Fillers

Theoretical predictions vs. experimental verifications

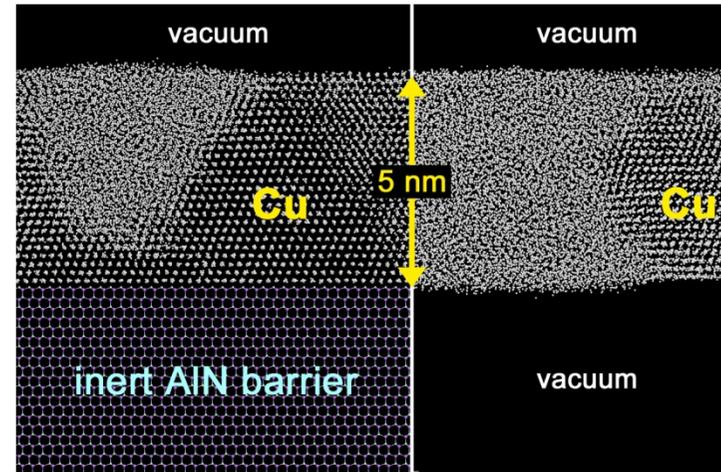


High-Resolution Transmission Electron Microscopy

Microstructural investigations by cross-sectional He-Focussed-Ion-Beam (FIB) imaging and HR-TEM



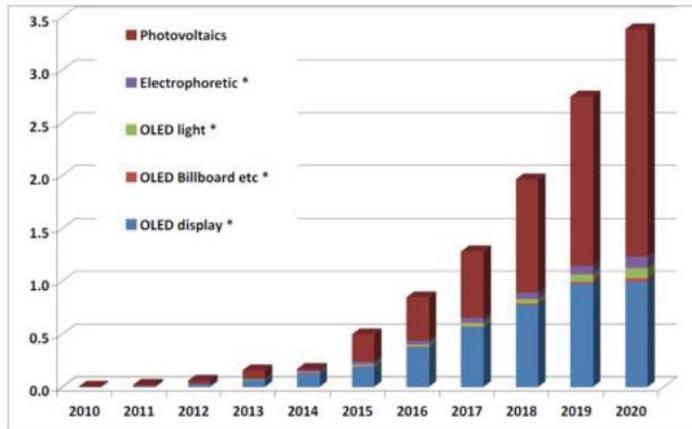
DFT and thermodynamic predictions of local interface structures and energetics



Multi-scale atomistic simulations (combining DFT, Molecular Dynamics, Monte Carlo, Molecular Statics) of pre-melting of free-standing and interface-bounded Cu films at 1200 K (bulk melting @1358 K).

Transparent Conductive Electrodes

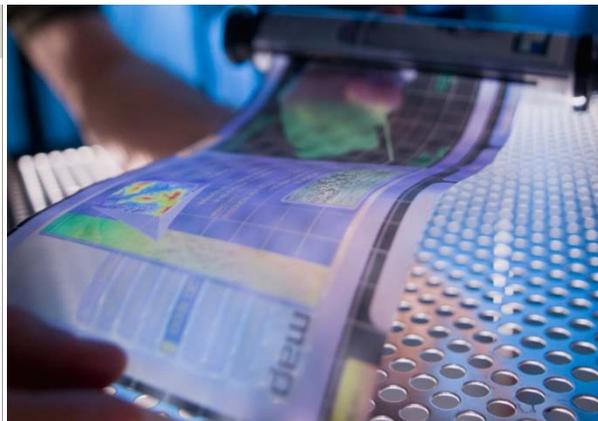
Applications of transparent conductive oxides (TCOs)



Source: IDTechEX



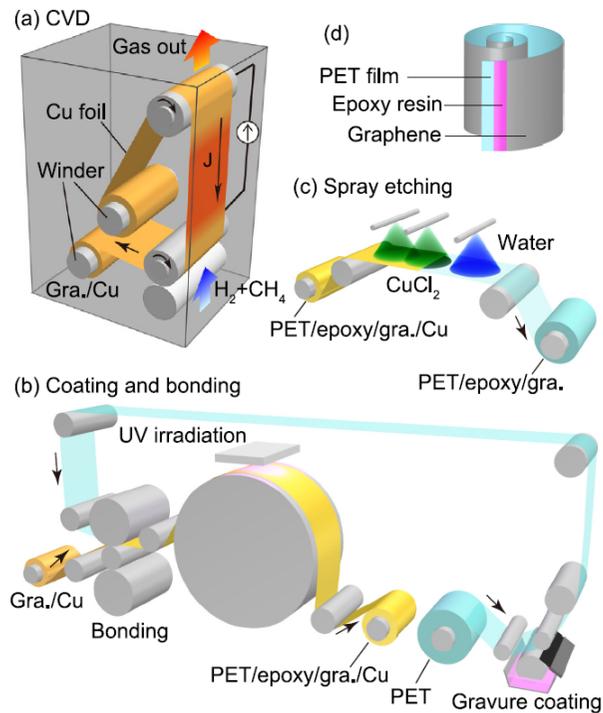
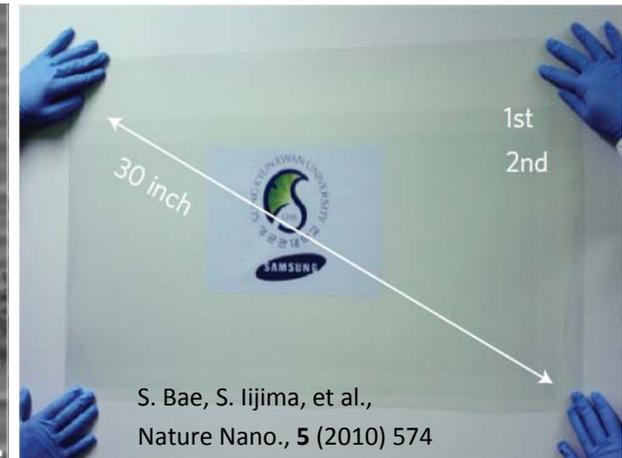
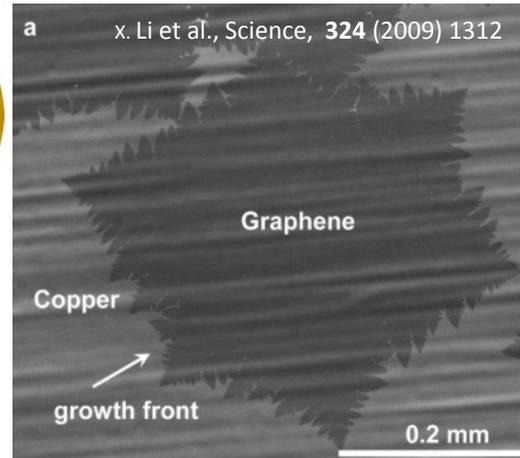
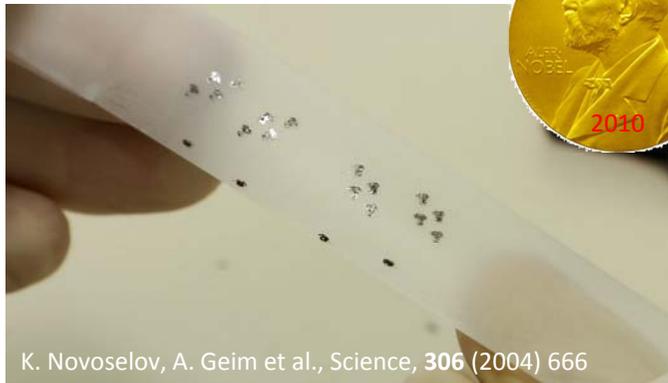
New applications: High flexible electronics (Prototypes of flexible computers (2013))



..... requires a replacement of TCOs. → Graphene is an excellent candidate!

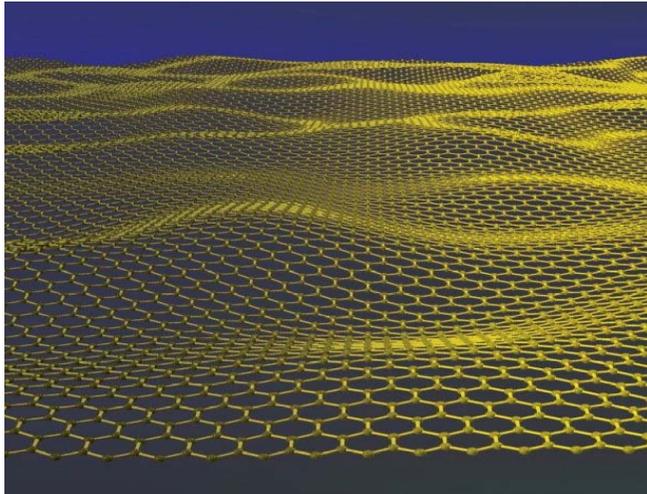
Graphene Synthesis

A Rapid Development

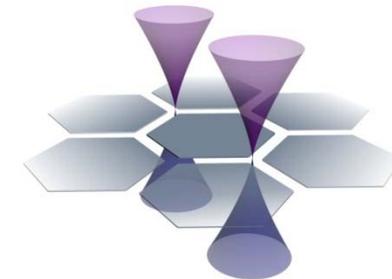


T. Kobayashi et al., Appl. Phys. Lett., **102** (2013) 023112

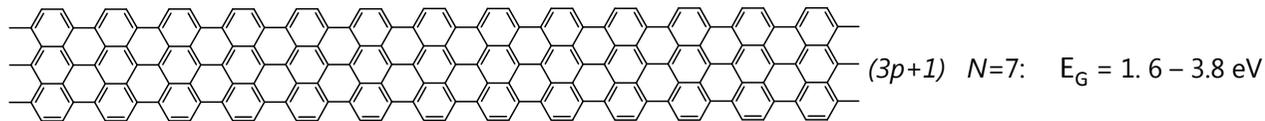
Graphene for Electronic Applications



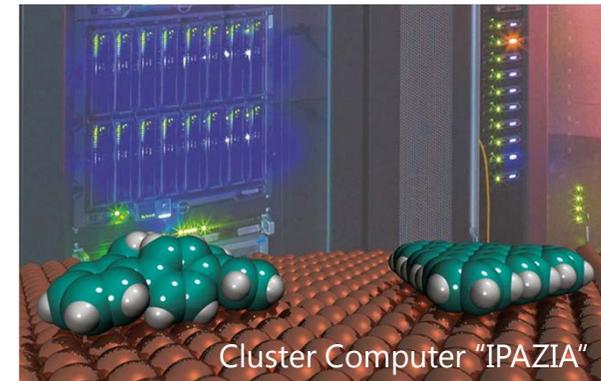
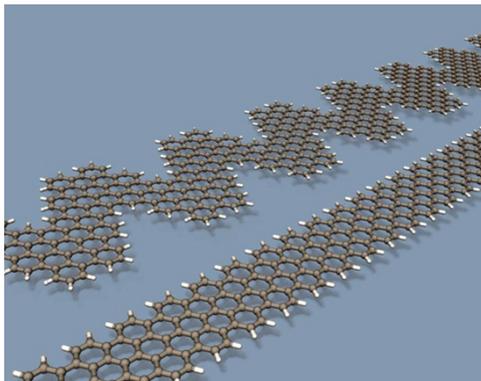
- ❑ Thermal conductivity:
 - ❑ Graphene $\sim 5000 \text{ Wm}^{-1}\text{K}^{-1}$
 - ❑ Silicon $\sim 150 \text{ Wm}^{-1}\text{K}^{-1}$
- ❑ Electron mobility:
 - ❑ Graphene $< 200'000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$
 - ❑ Silicon $1400 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$



Problem:
Graphene is a semi-metal and not a semi-conductor!!

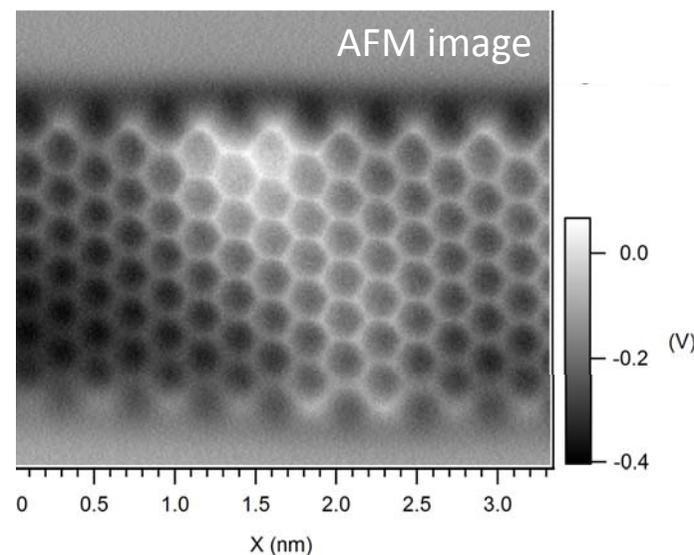
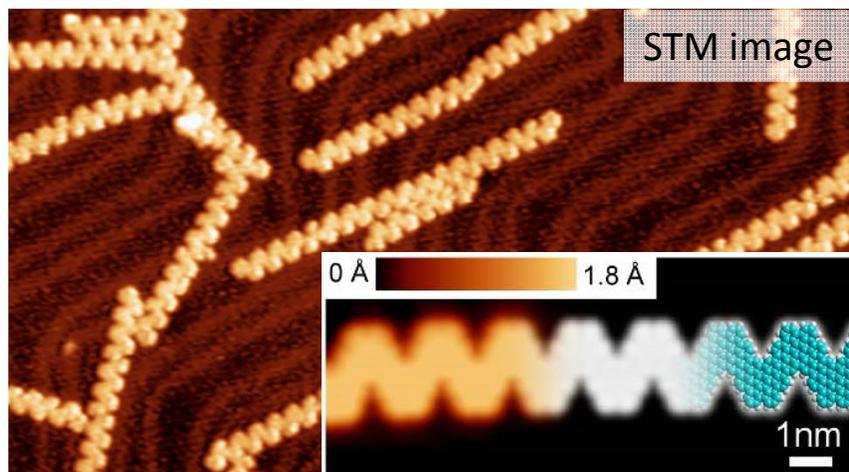
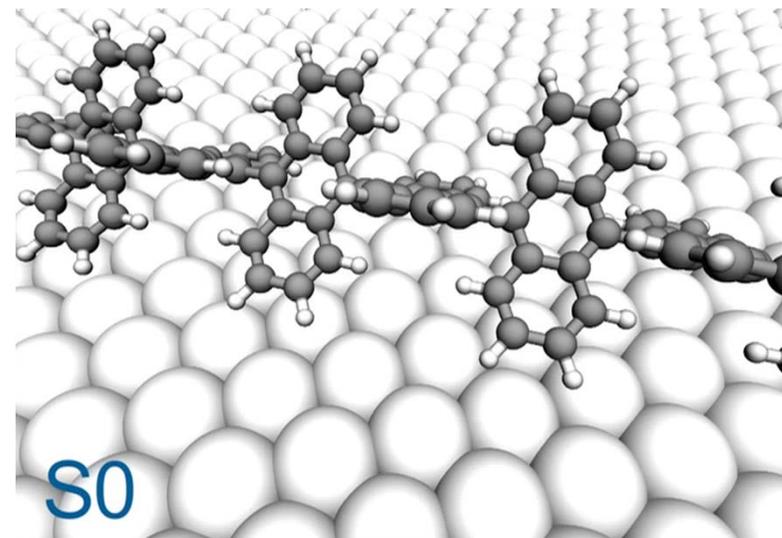
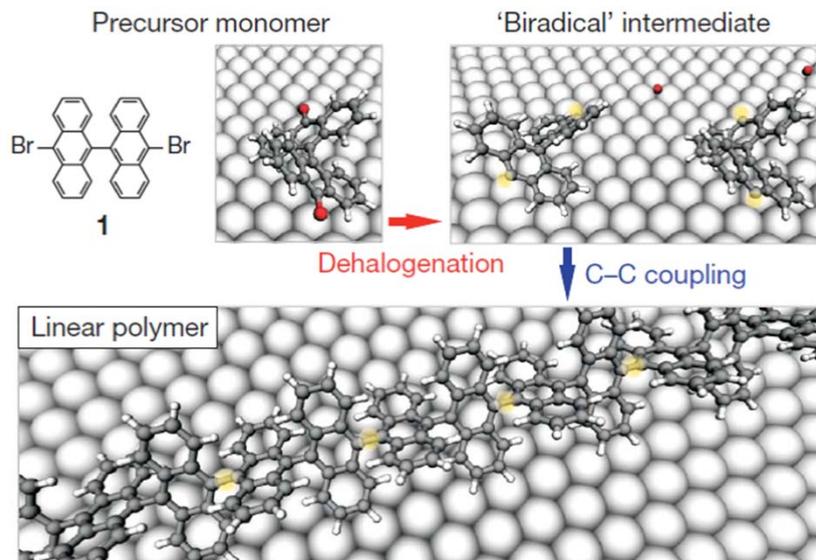


Theoretical prediction: Graphene Nanoribbons (GNR) are semiconductors!



Graphene Nanoribbons

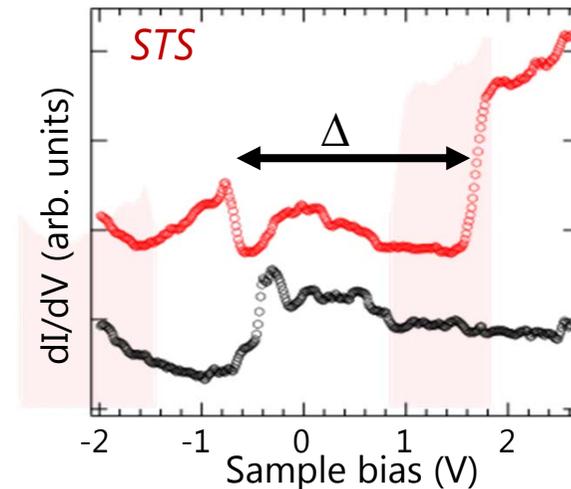
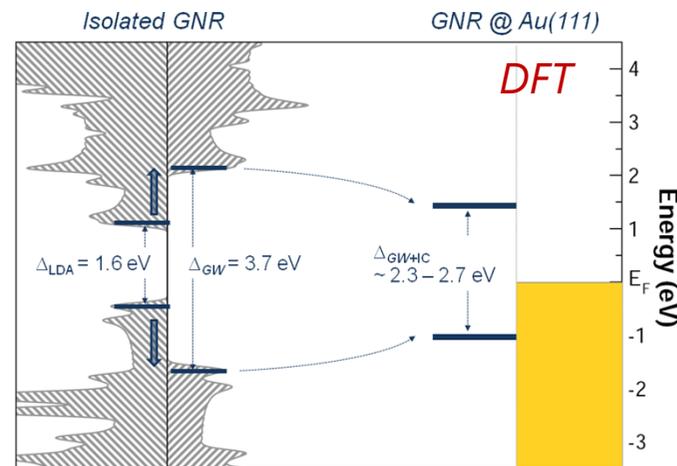
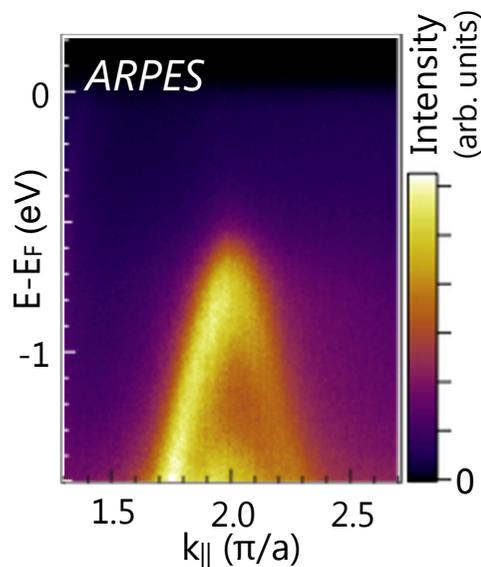
Bottom-Up Synthesis



"Nano-Structured Thin Films & Coatings"

Graphene Nanoribbons

- STS: band gap $\Delta = 2.3$ eV [on Au(111)]
- ARPES: $m^* = 0.21 m_0$; max. band slope: $8.2 \cdot 10^5$ m/s
- DFT: image charge correction of ~ 1.4 eV



Publications:

- Chem. Comm., 6919 (2009)
- JACS, **132**, 16669 (2010)
- Nature, **466**, 470 (2010)
- Nature Chem., **3**, 61 (2011)
- ACS Nano, **6**, 2020 (2012)
- ACS Nano, **6**, 6930 (2012)

..... the Material for Future Electronics!

*Thank you
for your
kind Attention*

