2D Materials Beyond Graphene For Future Electronics

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2D Materials – An (Incomplete) Overview

The most well-known 2D material: Graphene
- First 2D material studied in detail.
- Long history, finally became famous by the works of Novoselov & Geim and Berger & de Heer from 2004.
- High mobilities (>100 000 cm²/Vs @ 300K) raised expectations regarding electronic applications (possible successor of Si).
- European Graphene Flagship.

Meanwhile
- The prospects of graphene electronics are considered less optimistic.
- However, significant attention for 2D materials beyond graphene.
- So far, more than 500 layered materials discovered.
- Many of them semiconducting and possibly useful for electronics.
2D Materials – An (Incomplete) Overview

- Graphene, silicene, germanene
- Graphene nanoribbons (GNR)
- Bilayer graphene (BLG)
- Phosphorene, stanene

X-enes

MQ2: M = transition metal, Q = chalcogene (S, Se, Te)

- Mo-based TMDs, e.g., MoS2
- W-based TMDs, e.g., WS2

2D TMDs

2D Materials

X-anes
- Graphane
- Silicane
- Germanane
- Stanane

MX-enes
- M2X: M = early transition metal, X = C or N
- M2X plus F2, (OH)2, O2
e.g. Ti2CO2, Sc2CF2, ...

Many Further 2Ds
- Flouro-X-enes, Chloro-X-enes, SMCs,
- 2D III-Vs, 2D IV-IVs,
- 2D elementals, etc.
2D Materials – An (Incomplete) Overview

Conduction band
Bandgap $E_G$
Valence band

No gap, $E_G = 0$! This is really a pitty, since the missing gap causes serious problems for transistors.

Too narrow for logic transistors.

Many of these materials have a gap $E_G = 0.5...2.5$ eV, perfect for transistors.

X-enes
- Graphene
- Silicene
- Germanene

BLG

X-enes
- Phosphorene
- Stanene
- GNRs

MX-enes
- $\text{Sc}_2\text{CF}_2$
- $\text{TiCO}_2$

2D TMDs
- $\text{MoS}_2$, $\text{MoSe}_2$, $\text{MoTe}_2$
- $\text{WS}_2$, $\text{WSe}_2$, $\text{WTe}_2$

etc., etc.

Energy

Wave vector
Silicon rival MoS2 promises small, low-energy chips

The first computer chip made out of a substance described as a "promising" alternative to silicon has been tested by researchers.

The Switzerland-based team used molybdenite (MoS2) - a dark-coloured, naturally occurring mineral.

The group said the substance could be used in thinner layers than silicon, which is currently the most commonly used component in electronics.

The researchers say molybdenite microchips would need less power than existing silicon-based circuits.

http://www.bbc.co.uk/news/technology-16034693
How Promising are 2D Materials Beyond Graphene?

Graphene or Molybdenite? Which Replaces Silicon in the Transistor of the Future?
By Dexter Johnson
Posted 2 Feb 2011 | 19:25 GMT


‘Germanane’ may replace silicon for lighter, faster electronics

Germanane single- or multiple-atom-layer sheets can be exfoliated onto silicon dioxide or silicon surfaces (AFM image) (credit: Elisabeth Bianco et al./ACS Nano)

The chemists found that it conducts electrons more than ten times faster than silicon and five times faster than conventional germanium — the same material that formed the first primitive transistors more than 60 years ago

http://www.itpro.co.uk/635173/qa-what-will-wonder-material-graphene-give-us

Things seem to look good – TOO GOOD TO BE TRUE?
We should consider such statements very careful!
More Moore & More Than Moore

≈ 70 % of the overall chip market.

More Moore
- Compute
- Store
- Key enabler: CMOS scaling
- 2015: 16-nm gate MOSFETs, Si
- 2028: 5-nm gate MOSFETs
  Si, Ge, III-Vs
- Beyond 2028: < 5-nm gate MOSFETs
  Si, Ge, III-Vs, plus possibly 2D materials

More than Moore
- Interact with people + environment
- Exchange information
- Enhanced functionality
- 2015: Si, SiGe, GaAs, InP, GaN, SiC, ...
- 2028: Si, SiGe, GaAs, InP, GaN, SiC, ...
  plus most likely 2D materials
Trends In More Moore

- Moore’s Law: Doubling transistor count / chip every 18…24 months.
- Smaller transistors (scaling).

So far: Only one single device type – MOSFET.
So far: Only one single semiconductor – Si.
So far: Only one single technology – Si CMOS (complementary MOS, n-channel and p-channel Si MOSFETs).
The problem: An end of the Si MOSFET scaling is in sight!

Requirements for logic

- High on-off ratio $I_{on}/I_{off}$ ($10^4$...$10^7$).
- High $I_{on}$ (high speed).
- Low $I_{off}$ (low static power).
- Steep slope in sub-threshold, i.e., small SS.

Long channels: $I_{off} \propto \exp \left( \frac{-E_G}{m k_B T} \right)$

A sizeable gap is mandatory!
Trends in More Moore

High on-current $I_{on}$
- High carrier mobility $\mu$ needed, introduction of high-$\mu$ light-$m_{eff}$ channels.

Low off-current $I_{off}$ and small $SS$
- Good electrostatic integrity required to suppress short-channel effects, a short scale length $\lambda$ is beneficial.

$$\lambda = \sqrt{\frac{\varepsilon_{ch}}{\varepsilon_{bar}}} t_{ch} t_{bar}$$

$\lambda$ expression for single-gate SOI MOSFETs
Yan et al., TED 39, 1704 (1982).

Expressions for other MOSFET architectures (multi-gate, nanowire, 2Ds) have been elaborated.

In any case: Thin and narrow channel regions favorable. Introduction of ultra-thin body SOI, multi-gate, and possibly 2D MOSFETs.

- Suppression of direct source-drain tunneling.
  - Currently ($L \geq 10$ nm) not a problem.
  - Will become an issue at ultra-short gate length levels.
Trends In More Moore

A trend today: High-\(\mu\) channel materials for Si-based CMOS. Higher mobility to enhance on-current and transistor speed.

- Strained Si (sSi) with enhanced \(\mu\) & lower \(m_{\text{eff}}\).
- 2003: Intel introduced sSi into mass production.
- Today: All major chip-makers use sSi.

End of roadmap
- InGaAs nMOSFETs
- Ge p-MOSFETs again higher \(\mu\) again lower \(m_{\text{eff}}\)

- Expectation (ITRS 2013): High-\(\mu\) channel materials in production around 2018.
- InGaAs for nMOS.
- Ge for pMOS.

Past
- Si nMOSFETs
- Si pMOSFETs
- moderate \(\mu\)
- moderate \(m_{\text{eff}}\)

Today
- sSi nMOSFETs
- sSi pMOSFETs
- higher \(\mu\)
- lower \(m_{\text{eff}}\)
The hole mobility (not shown) exhibits a similar trend.

Regarding mobility, the 2D materials do not show a distinct advantage over the conventional 3D bulk materials. HOWEVER, ...

Electron mobility of different semiconductors vs bandgap.
Mobility

... However, to maintain good electrostatic integrity,

(i) UTB SOI MOSFETs (ultra-thin body)

(ii) Multiple-gate MOSFETs with narrow bodies, such as FinFETs, nanowire FETs, etc.

replace the conventional single-gate bulk MOSFET. Thin & narrow bodies reduced mobility.

FS, H. Wong, and Liou, Pan Stanford (2010).
Mobility

Severely degraded electron mobility in small-diameter Si nanowires.

The picture gets less cloudy for the 2Ds. The 2Ds are by nature ultimately thin.

A View Beyond the ITRS Horizon

• How far can the MOSFET be scaled? Unclear at present. Many problems: - Degraded electrostatics, degraded switch-off. - Variability and processing issues - Economic issues, cost.

• We remember: The 2013 edition of the ITRS requires 5-nm gate MOSFETs for the year 2028.

• One could say “5-nm MOSFETs – this is wishful thinking“, BUT the same has been said about 30-nm MOSFETs 20 years ago.

Monte Carlo Simulation of a 30 nm Dual-Gate MOSFET: How Short Can Si Go?

D. J. Frank, S. E. Laux and M. V. Fischetti
IBM Research Division, T. J. Watson Research Center
P.O. Box 218, Yorktown Heights, NY 10598

Note: In 1992, 500-nm single-gate MOSFETs have been in production.

• Production-stage 5-nm CMOS should not be ruled out. Let us be optimistic and assume the MOSFET can be scaled to sub-5-nm.
A View Beyond the ITRS Horizon

Meanwhile several theoretical studies on 5-nm gate MOSFETs:
- Luisier et al., IEDM, 251 (2011).
- Sylvia et al., IEEE TED 59 2064 (2012).
- Mehrotra et al., IEEE TED 60, 2171 (2013).
- etc.

• Consistent conclusion: At 5-nm and below gate lengths levels, source-drain tunneling will become an issue.

• Tunneling degraded SS and switch-off, high $I_{off}$.

• High-$\mu$, i.e., light-$m_{eff}$ narrow-gap channel materials are expected to fail.

• Heavy-$m_{eff}$ materials (with lower $\mu$ and wider gap) are expected to become favorable.
Our approach: Simple textbook expressions, critical input data from a more elaborated study (Sylvia et al.)

\[ TC = \left[ 1 + \frac{E_{\text{bar}}^2}{4E\left(E_{\text{bar}} - E\right)} \right]^{-1} \]

\[ k = \sqrt{2m_{\text{eff}}(E_{\text{bar}} - E)} / \hbar \]

\[ I_{\text{tun}} \approx c \times M \times TC \]

\( M \): Conduction band degeneracy factor 4 for Si and Ge NWs, 1 for III-V NWs.

\( c \): a constant, here 10.4 µA.

Our simplified approach reproduces the trend reported by Sylvia et al. nicely.
5-nm MOSFETs – Source-Drain Tunneling

NW(i): <110> Si, 3 GPa compressive strain.

NW(ii): <100> Si, 2 GPa compressive strain.

Si remains a strong contender!

m_{eff} for 3.8-nm Si NWs: Mehrotra et al., TED 60, 2171 (2013).

A possible scenario for the selection of MOSFET channel materials.

Past
Si nMOS
Si pMOS
Moderate μ
Moderate m_{eff}

Today
sSi nMOS
sSi pMOS
Higher μ
Lower m_{eff}

End of roadmap
III-V nMOS
Ge pMOS
Even higher μ
Even lower m_{eff}

Beyond roadmap
L ≤ 5 nm
2D or Si NWs or GNRs
Low μ
High m_{eff}
2D Transistors for More Than Moore – RF

Max. frequency of oscill. $f_{\text{max}}$ (GHz) vs. Cutoff frequency $f_T$ (GHz)

- InP HEMT & GaAs mHEMT
- Si MOSFET
- Graphene MOSFET
- MoS$_2$ MOSFET
- Phosphorene MOSFET

Pairs of numbers $f_{\text{max}}$, $f_T$:
- 1200, 600-700
- 800, 688
- 420, 360
- 325, 300
- 105, 93
- 70, 110
- 40, 150
- 20, 12


2D transistors
- Are definitely capable of RF operation.
- Cannot compete with high-performance III-V and Si RF transistors.
2D Transistors for More Than Moore – Flexible

Flexible Graphene FETs

Promising:
• Flexible Graphene FETs for RF
• Flexible TMD FETs for digital logic and RF

Applications for flexible electronics
Flexible 2D transistors perform VERY competitive!

The 2Ds are flexible – and it is more elegant and more reasonable to use a flexible-by-nature material for flexible electronics.
Metrology Needs for 2D Electronics

Processing 2D transistors and circuits (with the exception of starting material preparation) is based on the well-established Si technology. Thus, many metrology needs for 2D electronics are the same as those for Si technology. There are, however, several additional needs, such as

- Analysis of crystallographic structure of 2D layers (at atomic level).
- Identification of the layer number of 2D sheets.
- Accurate measurement of width, edge configuration, and bandgap of narrow GNRs.
- Correct extraction of the mobility of top-gated 2D MOS channels.
- Analysis of the properties of contacts metal – 2D materials (contact type, i.e., Schottky or Ohmic, contact resistance).
- Measurement of heat transport properties of 2D materials: thermal conductivity and thermal boundary resistance (between 2D materials and the substrate/insulator underneath).
Metrology Needs – GNR Gap vs Width

The bandgap of GNRs depends strongly on the ribbon width and the edge configuration!

GNR bandgap vs width.
FS, Pezoldt, Granzner, Nanoscale 2015.
For many 2D materials, the gap varies significantly when the number of layers changes.

Data compiled from the literature.
Conclusion

• The 2D materials are DEFINITELY promising for many applications.

• 2D MOSFETs for More Moore
  - No significant impact expected in the near to medium term, i.e., within the current ITRS horizon \((L > 5 \text{ nm})\).
  - Potential beyond the ITRS horizon \((L \leq 5 \text{ nm})\)
    - 2Ds offer short scale length and excellent electrostatics.
    - TMD and GNR MOSFETs: Efficient suppression of direct source-drain tunneling).

• 2D MOSFETs for More Than Moore
  - Promising (already in the near to medium term) for flexible electronics, both digital and analog/RF.
  - 2Ds promising for printable and transparent electronics.
Conclusion

Metrology Needs

• Many of the metrology needs for 2D electronics are the same as for Si technology.
• There are, however, several additional needs regarding
  - Crystallographic structure of 2D layers at the atomic level.
  - Layer number of 2D sheets.
  - Width, edge configuration, and bandgap of narrow GNRs.
  - Mobility of top-gated 2D MOS channels.
  - Properties of contacts metal – 2D materials (contact type,
  - Heat transport properties.

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