HETEROGENEOUS INTEGRATION ROADMAP

2019 Edition

Chapter 15: Materials and Emerging Research Materials

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The 2021 edition of this Chapter will be posted early in 2022; please check back (eps.ieee.org/hir) to replace this earlier version with the latest one.

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Chapter 15: Materials and Emerging Research Materials

This chapter is in preparation, and will be integrated into the Roadmap at Version 1.1, planned for the end of 2019. In its place is the following summary and a series of slides giving the current status of current materials, and emerging research materials, and some information that is relevant to the progress needed over the next 10 to 15 years.

Executive Summary

The focus of the **Materials section** is on the evolution of materials that can provide a wider range of properties for conductors, semiconductors and insulators to meet demands for lower cost, reduced power, higher thermal density and higher performance. It will address requirements identified by other HIR TWGs. The time horizon is for new materials that will be in production within 10 years. Supply chain requirements will be included in collaboration with the Supply Chain TWG.

The **Emerging Research Materials section** focus is on the revolution in materials required for new device types, and disruptive improvements that can replace the conductors, insulators, semiconductors and optical materials in current device architectures. The time horizon is for new materials that will be in volume production beyond 10 years and up to 25 years.

The scope of the Chapter includes:

- Supporting the HIR working groups with new materials required to meet the difficult challenges they identify.
- Enabling disruptive changes in capability of emerging devices such as quantum computing, biomedical systems, flexible electronics, etc., through novel materials.
- Expanding the range of properties available through new classes of composite materials combining novel matrix materials with nano-materials.

Defining the difficult challenges requires close collaboration with other TWGs both within and outside of this Roadmap.

Heterogeneous Integration Roadmap

Materials and Emerging Research Materials

TWG Chair: Bill Bottoms

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Materials and Emerging Research Materials Chapter Scope

The **Materials Sub-chapter** focus is on the evolution of materials providing a wider range of properties for conductors, semiconductors and insulators to meet demands for lower cost, reduced power, higher thermal density and higher performance. The Scope will address requirements identified by other HIR TWGS. The time horizon is for new materials that will be in production within 10 years. Supply chain requirements will be included in collaboration with the Supply Chain TWG.

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Defining the difficult challenges requires close collaboration with other TWGs both in and outside of HIR.

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Heterogeneous Integration by Materials

Conductors
- Nanomaterials (CNT, graphene, nanowires)
- Metals (Cu, Al, W, Ag, Co, etc.)
- Composites

Dielectrics
- Oxides
- Polymers
- Porous materials
- Composites

Semiconductors
- Elemental (Si, Ge)
- Compounds (IIIV, IIVI, tertiary)
- Polymers

Materials Parameters must be compatible with each other for processing and operation:

- ✓ Cost
- ✓ CTE differential
- ✓ Thermal conductivity
- ✓ Fracture toughness
- ✓ Modulus
- ✓ Processing temperature
- ✓ Interfacial adhesion
- ✓ Operating temperature
- ✓ Breakdown field strength

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Difficult Materials Challenges 2019-2029 (1)

Materials and Emerging Research Material Difficult Challenges

Difficult Challenges 2018-2028	
Achieving desired properties in integrated structures	Identify integrated high k dielectrics with Equivalent Oxide Thickness <0.5nm, high breakdown field and low leakage
	Identify integrated contact structures that have ultralow contact resistance
	Achieving high hole mobility indirect band gap materials in FET structures
	Achieving high electron mobility in Ge with low contact resistance in FET structures
	Achieving a bandgap in graphene suitable for FET structures
	Multiferroic with Curie temperature >400K and high remnant magnetization to >400K
	Synthesis of single wall CNTs with tight distribution of bandgap and mobility
	Electrical control of the electron correlation, ex. Mott transition, Spin dynamics
	Simultaneously achieve package polymer CTE, modulus, electrical, thermal properties, with moisture and ion diffusion barriers for low stress packaging at use case temperature
	Thermal interface materials with low interface thermal resistance and high thermal conductivity with desired electrical and mechanical properties.
	Nanosolders compatible with <200C assembly, multiple reflows, high strength, high thermal and electrical conductivity and high electromigration resistance.
	NanoInks that can be printed as die attach adhesives with required electrical, mechanical, thermal, interface,and reliability properties.
	NanoInks that can be printed as conductors, via hole fillers, solders, or die attach adhesives with required electrical, mechanical, thermal, interface and reliability properties.

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Difficult Materials Challenges 2019-2029 (2)

Characterize and control coupled properties of embedded materials and their interfaces	High mobility transition metal dichalcogenides TMD with unpinned Fermi level and low resistance ohmic contacts.
	High electron mobility in Ge with unpinned Fermi level and low resistance ohmic contacts.
	High mobility nanowires with unpinned Fermi level and low interface resistance.
	Graphene with a bandgap suitable for FET structures, high mobility, and unpinned Fermi level at dielectric interfaces.
	Complex metal oxides with unpinned Fermi levels
	Characterization of electrical properties of molecule / metal contact interfaces (i.e. Pentacene/Au)
	Characterization of electrical properties of embedded nano contact interfaces (i.e. CNT/Metal)
	CNTs with low resistance contacts on both ends
	Characterization for density of dislocations and anti-phase boundary generating interface between Ge/III-V channel materials and Si.
Identifying manufacturable methodologies to enable deterministic fabrication with required property control	Dopant placement and activation i.e. deterministic doping with desired number at precise location for Vth control and S/D formation in Si as well as alternate materials.
	HVM compatible methods to place dopants in predetermined positions with minimal damage to the semiconductor.
	Manufacturing and purification methodologies of single wall CNTs to achieve required purity levels (pure semiconductor with bandgap)
	Identify DSA process simplification methodologies that can achieve required overlay requirements.
	Wafer scale growth of high quality graphene with desired process conditions (ex. Low temperature growth on metal or insulator)
	Controlling edge-termination / molecular absorption to graphene to achieve required bandgap.
	Synthesis or assembly of CNTs in predefined locations and directions with controlled diameters, chirality and site-density.
	III-V: Correlation between antiphase domains and electrical properties.
	Control defects in carbon nanotubes.
	Control defects in growth and processing of graphene.
	Control concentration and locations of cation and anion defects in complex metal oxides.
	Control precipitation in ferromagnetic semiconductors.
	Characterization for density of dislocations and anti-phase boundary generating interface between Ge/III-V channel materials and Si.

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Difficult Materials Challenges 2019-2029 (3)

	Si.
Control of Self-assembly processes to achieve desired properties reproducibly	Biocompatible functional materials
	DSA for Litho Extension: Efficient CAD models to enable translating design features to guide structures on photomasks.
	DSA for Litho Extension: Registration of self-assembled patterning materials in desired locations with control of geometry, conformation, interface roughness, and defects
	DSA for Litho Extension: Achieve realistic device pattern with reduced pattern roughness and defects
	Demonstrate self assembly's ability to deterministically control locations of dopants conformally on 3D structures

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Difficult Materials Challenges 2029-2043 (1)

Difficult Challenges 2029-2043	
Electric field control of the electrochemical reaction in a nanoscaled device and at an interface	Complex Oxides: Control of oxygen vacancy formation at metal interfaces and interactions of electrodes with oxygen and vacancies
	Switching mechanism of atomic switch: Improvements in switching speed, cyclic endurance, uniformity of the switching bias voltage and resistances both for the on-state and the off-state.
	Nano-Carbon / metal functional junction, such as new switch, by using electrochemical reactions
	Molecular device fabrication with precise control using electrochemical reactions
Metrology to characterize structure and properties of materials at the nanometer scale	Development of the method to evaluate the validity of the measurement result for each ERM
	Electrical and thermal properties of each carbon nanotube
	Nanowire characterization of mobility, carrier density, interface states, and dielectric fixed charge effects
	Graphene and TMD mobility and carrier concentration
	Complex metal oxide characterization of carrier density, dielectric and magnetic properties
	Spin materials: characterization of spin, magnetic and electrical properties and correlation to nanostructure
	Characterization of electrical properties of embedded nano contact interfaces (ex. CNT/Metal)
	Evaluating material properties in realistic device structures
	Nanoscale observation of the magnetic domain structure, for example, the domain in STT-RAM under the magnetic field, i.e., the dynamic operation

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Difficult Materials Challenges 2029-2043 (2)

Metrology to characterize defects at the nanometer scale with atomic resolution	Nanowires: Characterization of vacancies, interstitials and dopants within the NW and at interfaces to dielectrics
	Graphene: Characterization of edge defects, vacancies and interstitials within the material and at interfaces
	Metal nanoparticles: Native oxide interface and crystal defects in the nanoparticle
	Complex Oxides: Location of oxygen vacancies and the valence state of the metal ions
	Spin materials: characterization of vacancies in spin tunnel barriers, and defects within magnetic materials and at their interfaces
	Evaluating material properties IN realistic nm scale devices
	Characterization of edge structure and termination with atomic resolution (ex. Graphene nano ribbon, TMD, etc.)
Accurate multiscale simulation for predictions of unit processes the resulting structure, properties and device performance.	Linkage between different scales in time, space, and energy bridging non-equilibrium phenomena to equilibrium phenomena
	Transferable simulation tools for many kinds of materials
	Development of platform for different simulation tools, such as TCAD and ab-initio calculations
	Nanowires: Simulation of growth and defect formation within and at interfaces
	CNTs: Simulation of growth and correlation to bandgap
	Graphene: Simulation of synthesis, edge defects, vacancies, interstitials, interfacial bonding, and substrate interactions.
	Atomistic simulation of interfaces for determining Fermi level location and resulting contact resistivity
	Nanoparticles: Simulation of growth and correlation to structure and defects
	Complex Oxides: Multiscale simulation of vacancy formation, effect on metal ion valence state and effect of the space charge layer
	Spin: Improved models for multiscale simulation of spin properties within materials and at their interfaces.

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Difficult Materials Challenges 2029-2043 (3)

Fundamental thermodynamic stability and fluctuations of materials and structures	Geometry, conformation, and interface roughness in molecular and self-assembled structures
	Device structure-related properties, such as ferromagnetic spin and defects
	Dopant location and device variability
Materials and processes that enable monolithically integrated complex functionality	Integration on CMOS Platforms
	Integration with flexible electronics
	Biocompatible functional materials
	Robust long-term biotic-abiotic interfaces that avoid biofouling isses
	Leveraging convergent materials experetise in adjacent sectors

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Work in Progress. Please do not distribute without permission of HIR IRC

New Conductors and Joining Processes Have Been Known For Years But Are Not Yet Used In Volume Production

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Warpage For Ever Thinner Layers

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Solutions for warpage are known and demonstrated but not integrated for production

- Reduced copper CTE (4.5 rather than 17)
- Low-modulus dielectrics
- No underfill
- Direct interconnect bonding
- All joining processing done at or near use-case temperature

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Warpage For Ever Thinner Layers

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Combining These Materials And Processes Solves Stress and Warpage Issues And Improves Performance

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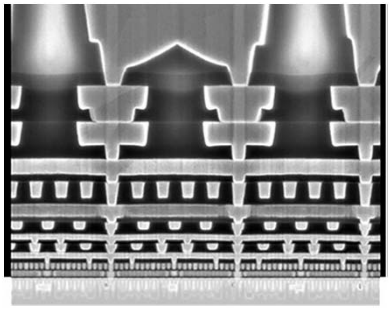
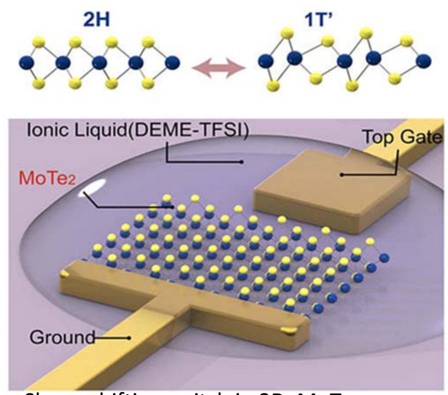
Examples Of New Materials With Proof Of Concept



Cobalt & Cobalt/Copper, in use today.
Contact resistance reduced 1.5X,
Line resistance down 60%. Intel



Shape shifting switch in 2D $MoTe_2$
X . Zhang, Berkeley

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Thermal Management

Key elements of thermal management

- Don't make heat in the first place (device design, low frequency-high parallelism, subthreshold operation, reduced interconnect distance)
- Lower-resistance conductors
- Lower operating voltage
- Lower-k dielectrics
- Active voltage control
- Rapid shut down and power up (sub-nanosecond. GaN)
- Improved heat sink materials and design

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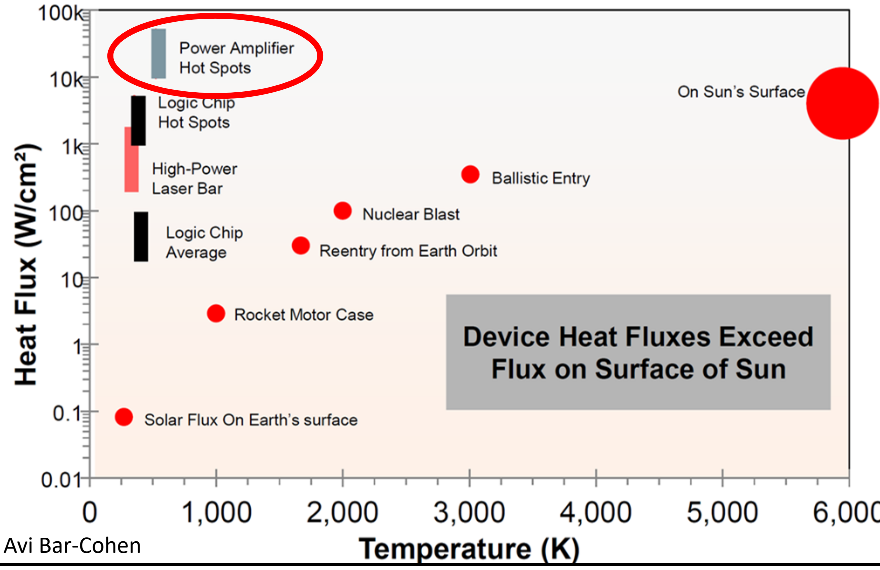
Thermal Management Reaching Limits of Imagination



Source: Raytheon, Avi Bar-Cohen

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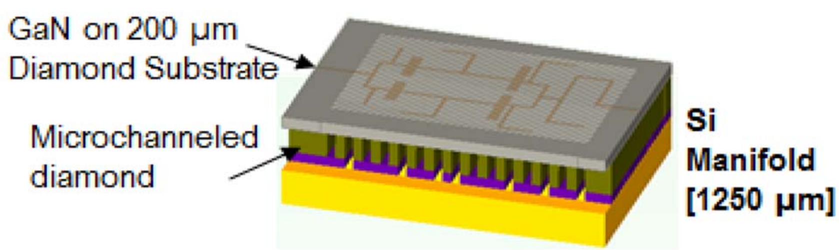
Diamond Microchannel Bonded to GaN Amplifier



GaN-on-Diamond with diamond microchannels and wafer-bonded Si microchannel liquid manifold

Source: Raytheon, Avi Bar-Cohen

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This System Is In Operation At 10KW/cm^2

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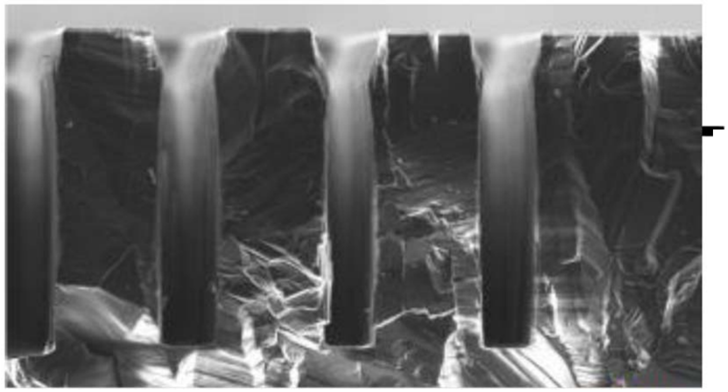
Forming of High Aspect Ratio Micro-channels in Diamond



Source: Raytheon, Avi Bar-Cohen

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Examples Of Materials Requirements For The Next Quarter Century

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New materials for replacing the CMOS switch

- 2D materials: perhaps CNT and graphene similars made of other atoms
- Nano-wires for interconnect and device switch structures
- Conductors that can be used for atomic level mechanical switch
- Optical switch material supporting all-optical logic
- Biomaterials for “brain” energy-level switch
- Biomaterials for self assembly in complex interconnect systems
- Things we cannot yet imagine

The 25 year horizon includes more than development of the materials. Equipment, processes and supply chain must be in place to support volume production.

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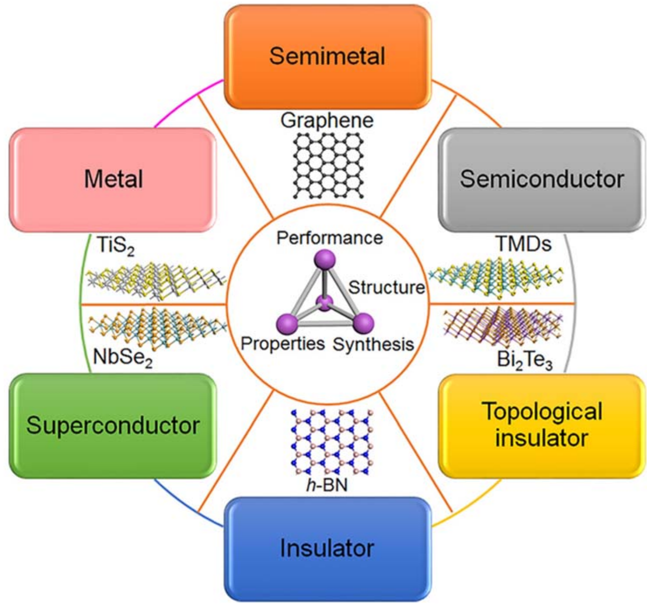
2D Class Of Materials Can Support Many Device Types



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Nano-Infused Ceramic Self-Report For Self-reporting Structural Sensors (Composite Materials)

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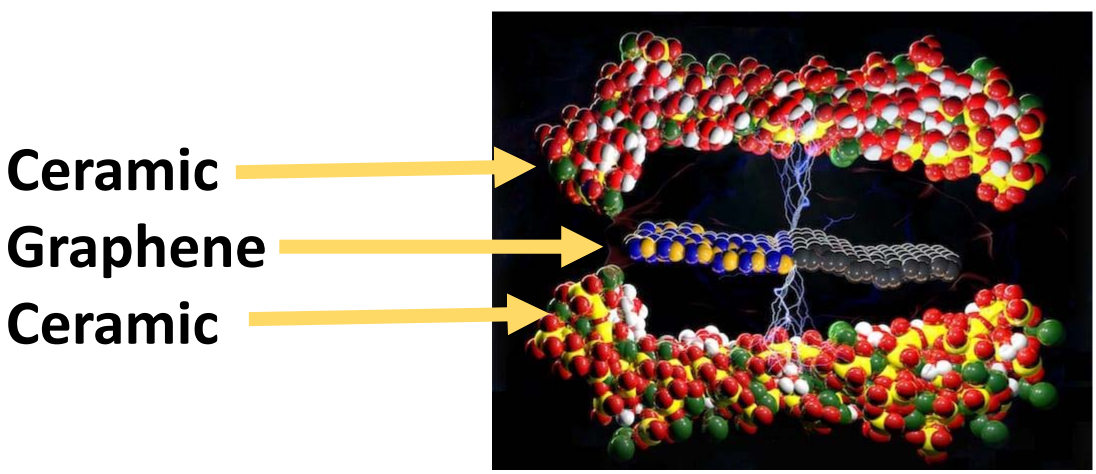

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Artificial Intelligence May Design New Materials

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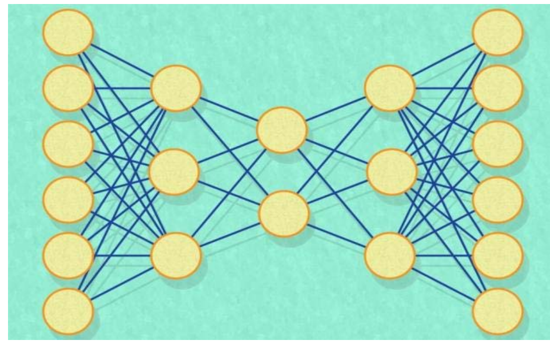
The MIT system uses statistical methods that provide a natural mechanism for generating original recipes, which suggest alternative recipes for known materials that accord well with real recipes.

AI and Big Data can learn to design applications specific materials



A machine-learning system analyzes materials "recipes" using an autoencoder. If successfully trained, the system will capture the data's characteristics. Image: Chelsea Turner/MIT

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Summary

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- The Materials Sub-chapter identifies difficult challenges and potential solutions and identifies probable date for volume production in our Tables for selected examples.
- The Emerging Research Materials Sub-Chapter identifies difficult challenges and, where possible, potential solutions for selected examples. There is no prediction of the date for volume production.

Our objective is to accelerate the pace of progress by stimulating pre-competitive collaboration.

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