Unique Properties of Quasi-One-Dimensional van der Waals Materials and Heterostructures

Alexander A. Balandin

Nano-Device Laboratory: NDL
Center for Phonon Optimized Engineered Materials: POEM
Department of Electrical and Computer Engineering
Materials Science and Engineering Program
University of California – Riverside

CONTROL ID: 3330101
PRESENTATION TYPE: Invited Speaker
Symposia: S.EL02: Advanced Manufacturing of Mixed Dimensional Heterostructures

MRS Invited – November 2020

| Nano-Device Laboratory >

UNIVERSITY OF CALIFORNIA
UC RIVERSIDE


City of Riverside


UCR Bell Tower


UCR Engineering Building


UCR Botanic Gardens


Joshua Tree Park

Funding Acknowledgement

National Science Foundation (NSF) program Designing Materials to Revolutionize and Engineer our Future (DMREF) via a project DMR-1921958 entitled Collaborative Research: Data Driven Discovery of Synthesis Pathways and Distinguishing Electronic Phenomena of 1D van der Waals Bonded Solids
UCR PI: A.A. Balandin, Co-PI: L. Bartels; Stanford Lead PI: E. Reed

Semiconductor Research Corporation (SRC) contract 2018-NM-2796 entitled One-Dimensional Single-Crystal van-der-Waals Metals: Ultimately-Downscaled Interconnects with Exceptional Current-Carrying Capacity and Reliability
UCR PI: A.A. Balandin, Co-PI: L. Bartels

NSF DMR Major Research Instrumentation (MRI): Development of a Cryogenic Integrated Micro-Raman-Brillouin-Mandelstam Spectrometer
UCR PI: A.A. Balandin, Co-PI: F. Kargar

Outline of the Talk

→ Definition: Quasi-1D van der Waals materials

→ Motivations

→ Properties

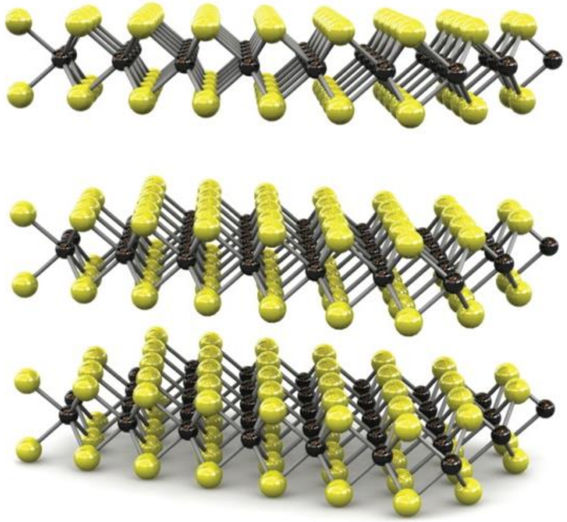
→ Current conduction of quasi-1D bundles

→ Electromagnetic interference shielding of composites with quasi-1D materials

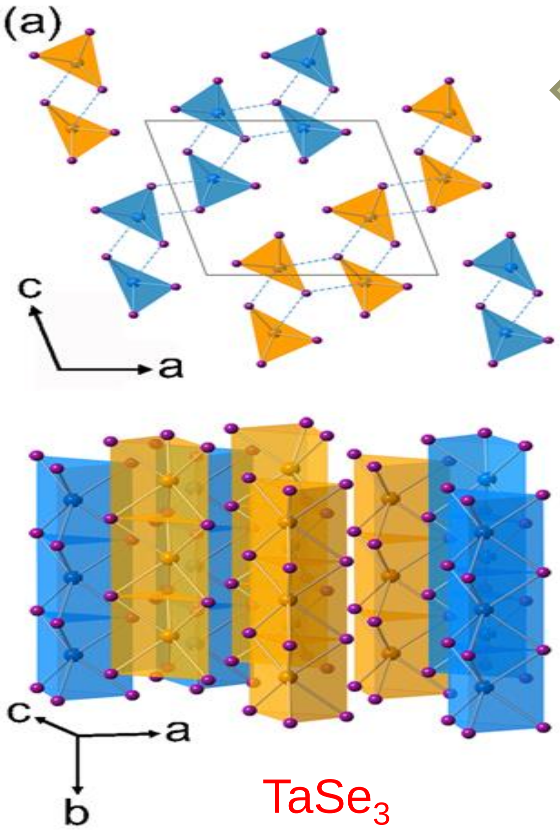
→ Conclusions

Terminology: Van der Waals Materials

Quasi-2D van der Waals Materials



MoS_2



$TaSe_3$

atomic threads

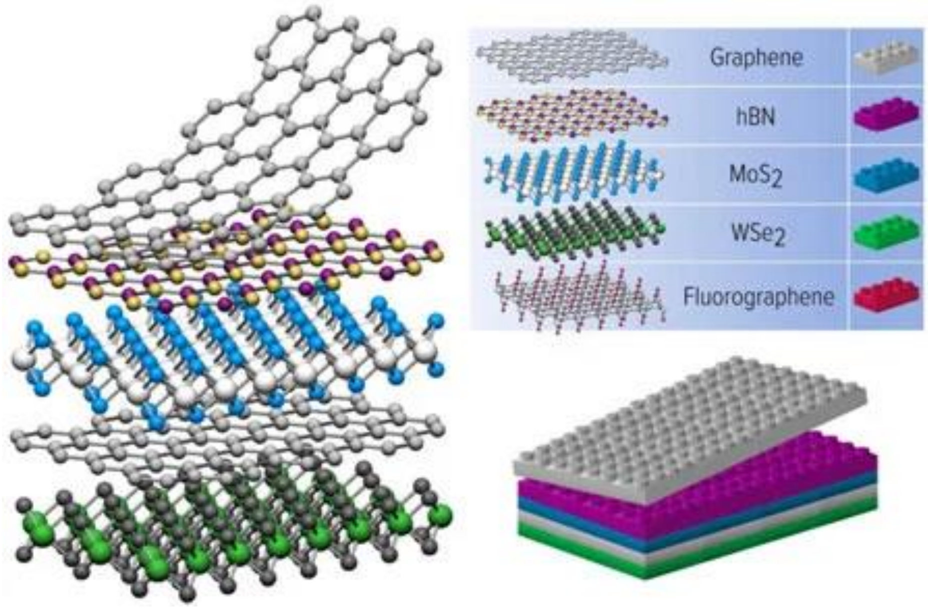
Quasi-1D van der Waals Materials

→ Crystal structure of monoclinic $TaSe_3$, with alternating layers of $TaSe_3$

→ Cross section of the unit cell, perpendicular to the chain axis (b axis).

→ The side view: 1D nature of $TaSe_3$ chains along the b axis.

Concept of 1D and Quasi-1D



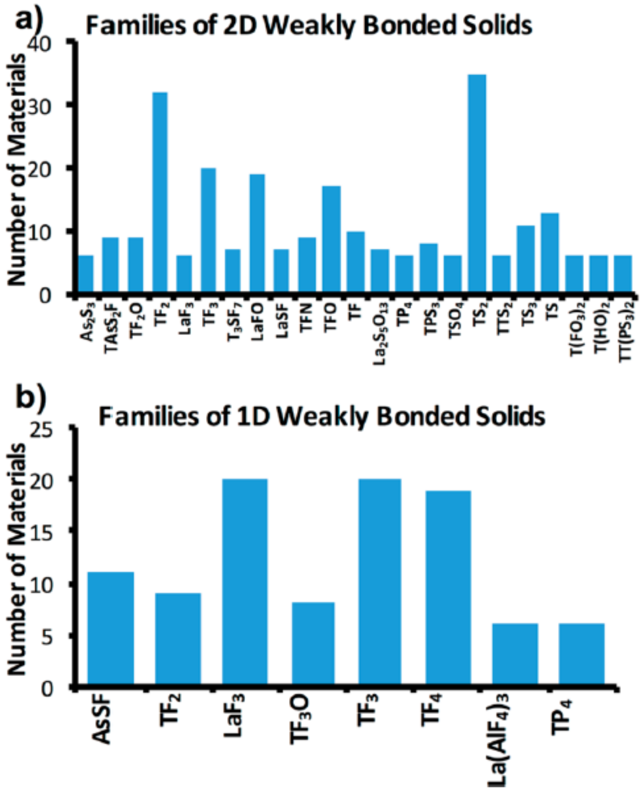
A. K. Geim and I. V. Grigorieva
Nature, 499, 419 (2013)

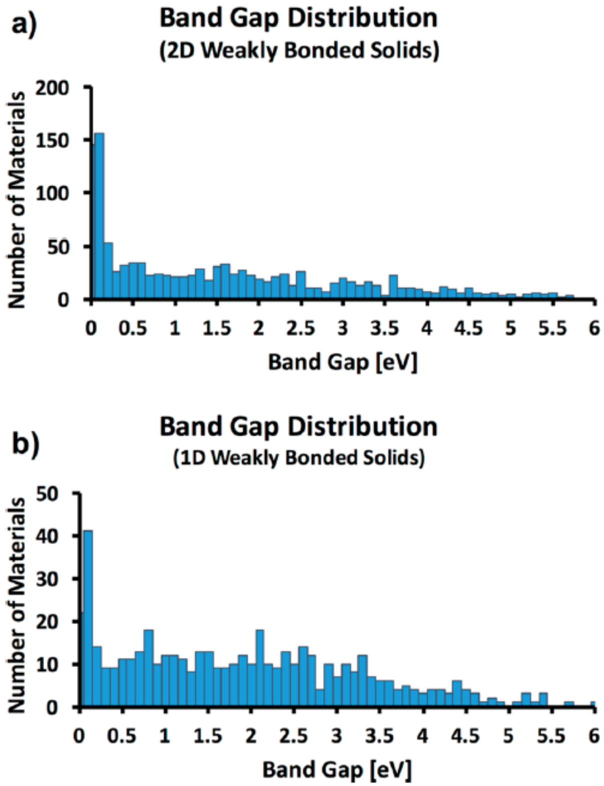
2D → 1D

UC Riverside

Large Library of 1-D van der Waals Materials

Reed Group, Stanford





There are numerous 1D and quasi-1D van der Waals materials with the wide range of bandgaps and effective masses.

G. Cheon, et al., “Data Mining for New Two- and One-Dimensional Weakly Bonded Solids” Nano Letters 17, 1915 (2017).

NSF DMREF Stanford – UCR Project

The Meaning of “Quasi” and “Quantum”

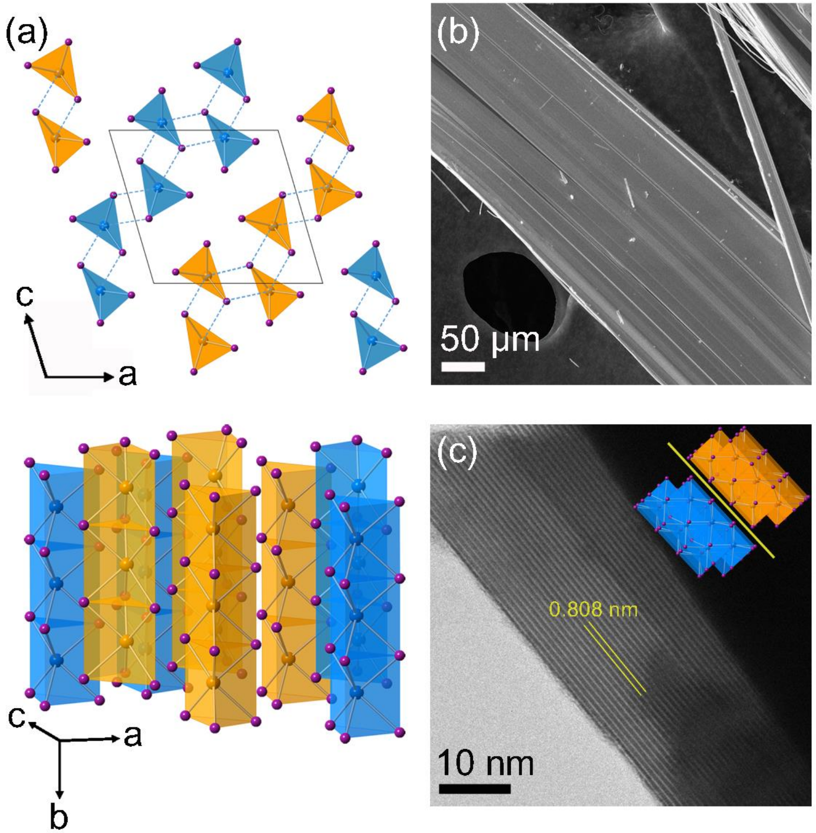
→“Quasi” in a sense of a bundle

→“Quasi” in a sense that you may have weaker covalent bonds in perpendicular plane

→ $ZrTe_3$ is in between 2D and 1D material

→ “Quantum” in a sense of quantum confinement: it can reveal itself differently for van der Waals materials

→ “Quantum” is relation to the charge-density-wave phases

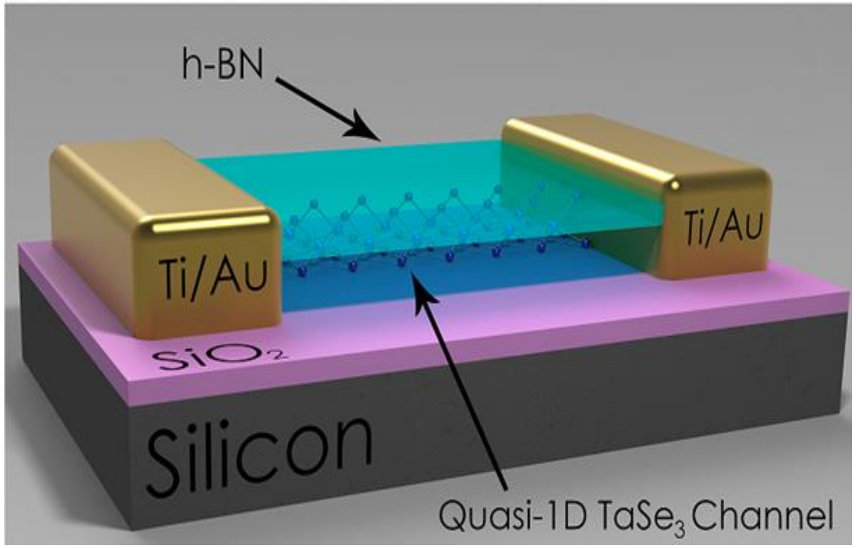


At this point, we work with bundles, not individual chains

$TaSe_3$

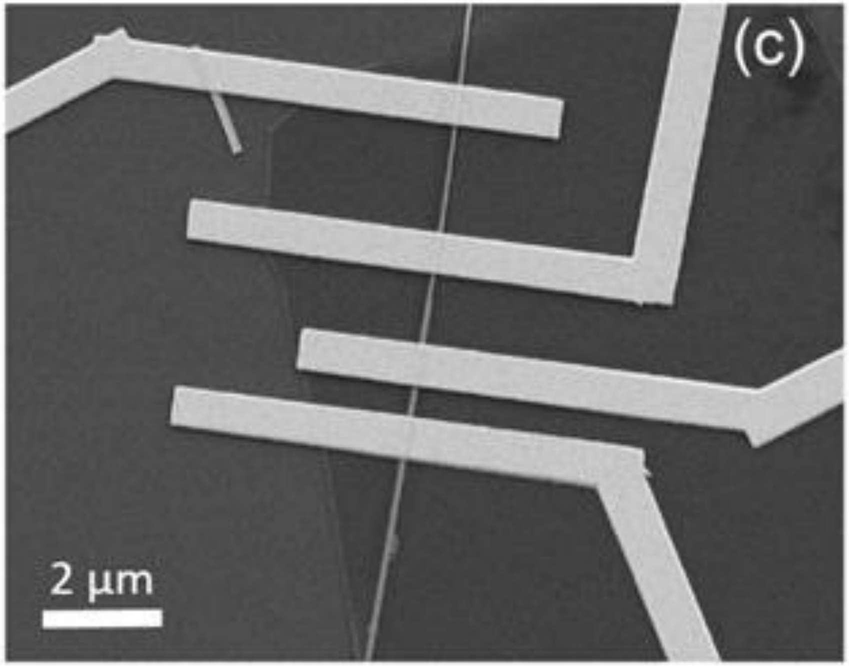
Quasi-1D Channel $TaSe_3$ Devices Fabricated by Electron Beam Lithography

Quasi-1D bundles and BN capping



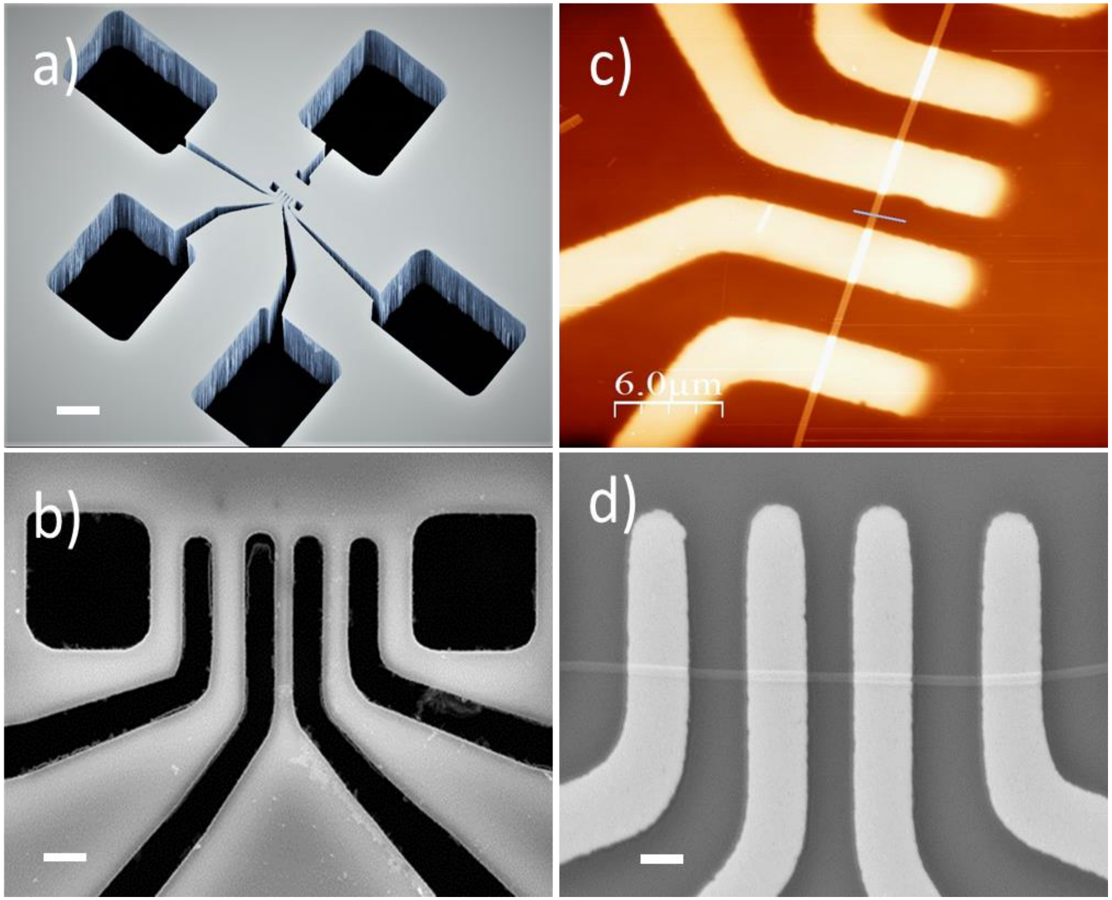
Schematic of the $TaSe_3$/h-BN quasi-1D / quasi-2D nanowire heterostructures used for the I-V testing.

Range: 20 nm to 100 nm



The metals tested for fabrication of Ohmic contacts included combinations of thin layers of Cr, Ti, Au, Pd together with a thicker Au layer.

Quasi-1D Channel $ZrTe_3$ Devices Fabricated by Shadow Mask Method



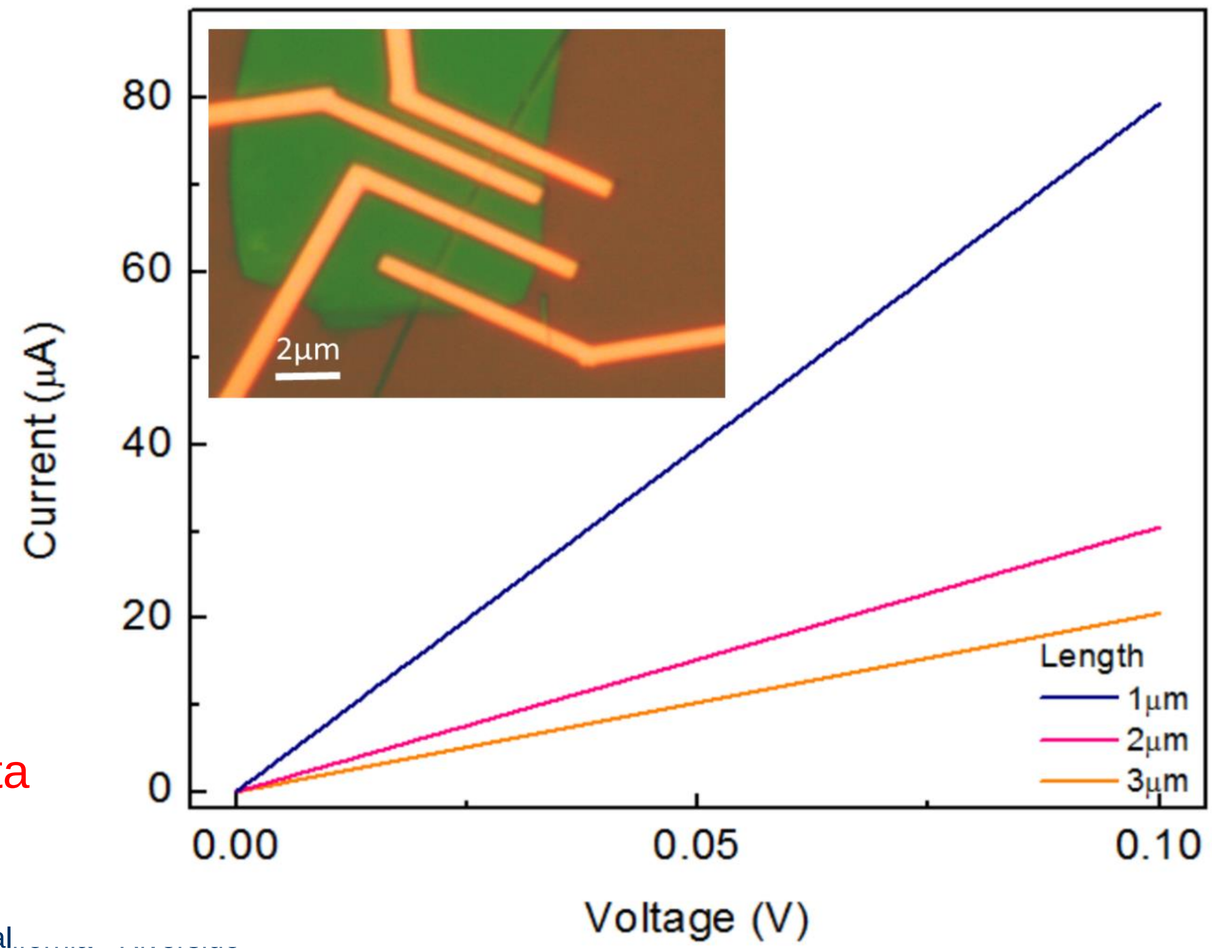
(a) SEM image of a shadow mask. (b) SEM image of the pattern for Ti and Au evaporation to create the contacts. (c) AFM image of the quasi-1D $ZrTe_3$ nanoribbon device. AFM characterization was used to determine the nanowire width and thickness (33-nm in the present case). (d) SEM image of another quasi-1D ZrTe3 nanowire device with a different cross-sectional area. The scale bars in (a), (b) and (d) are 50 µm, 2 µm and 1 µm respectively.

Electrical Characteristics of Devices with Quasi-1D $TaSe_3$ Channels – Ohmic Contacts

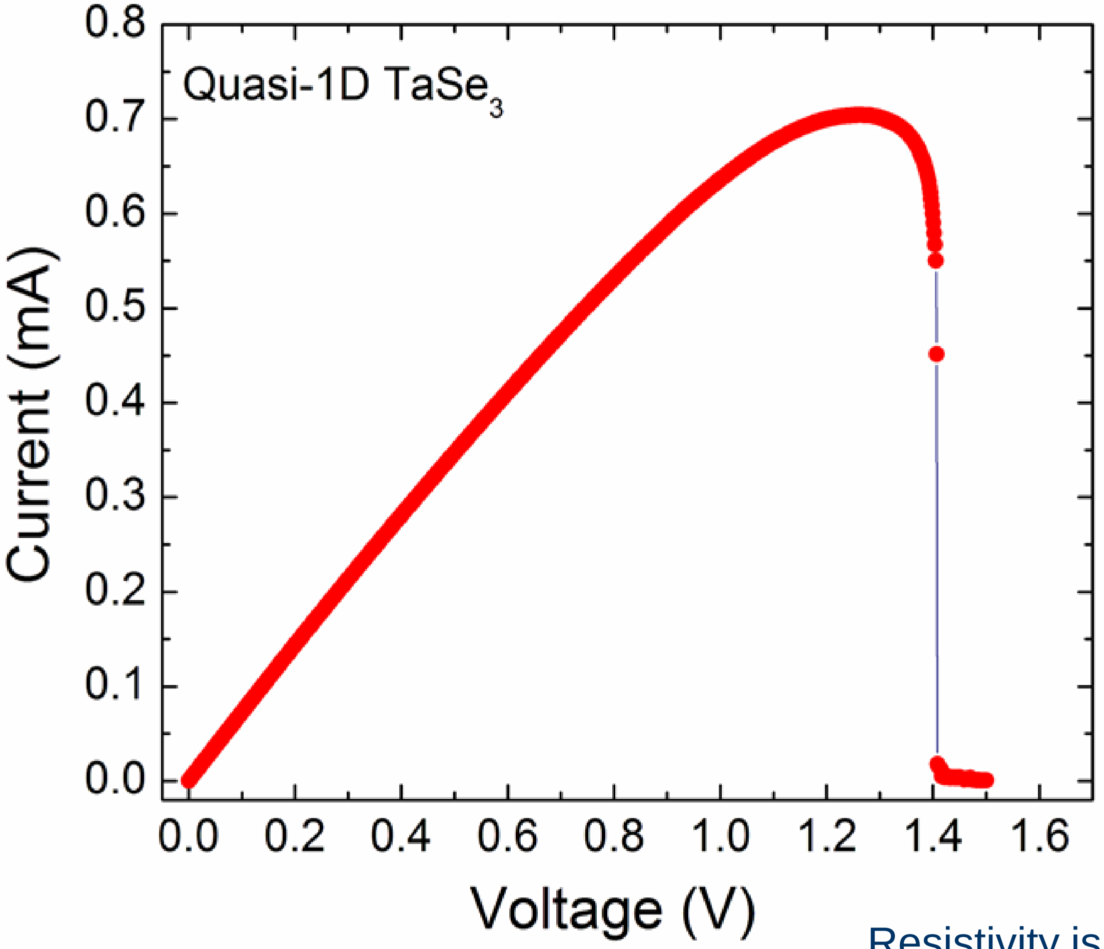
→ Current-voltage characteristics of $TaSe_3$ devices with different channel length.

→ Linear characteristics at low voltage indicates good Ohmic contact of $TaSe_3$ channel with the metal electrodes.

The contact resistance extracted from TLM data is $2R_C$=22 Ω-μm



Current Density in Quasi-1D $TaSe_3$ Nanowires – Bundles of Atomic Chains



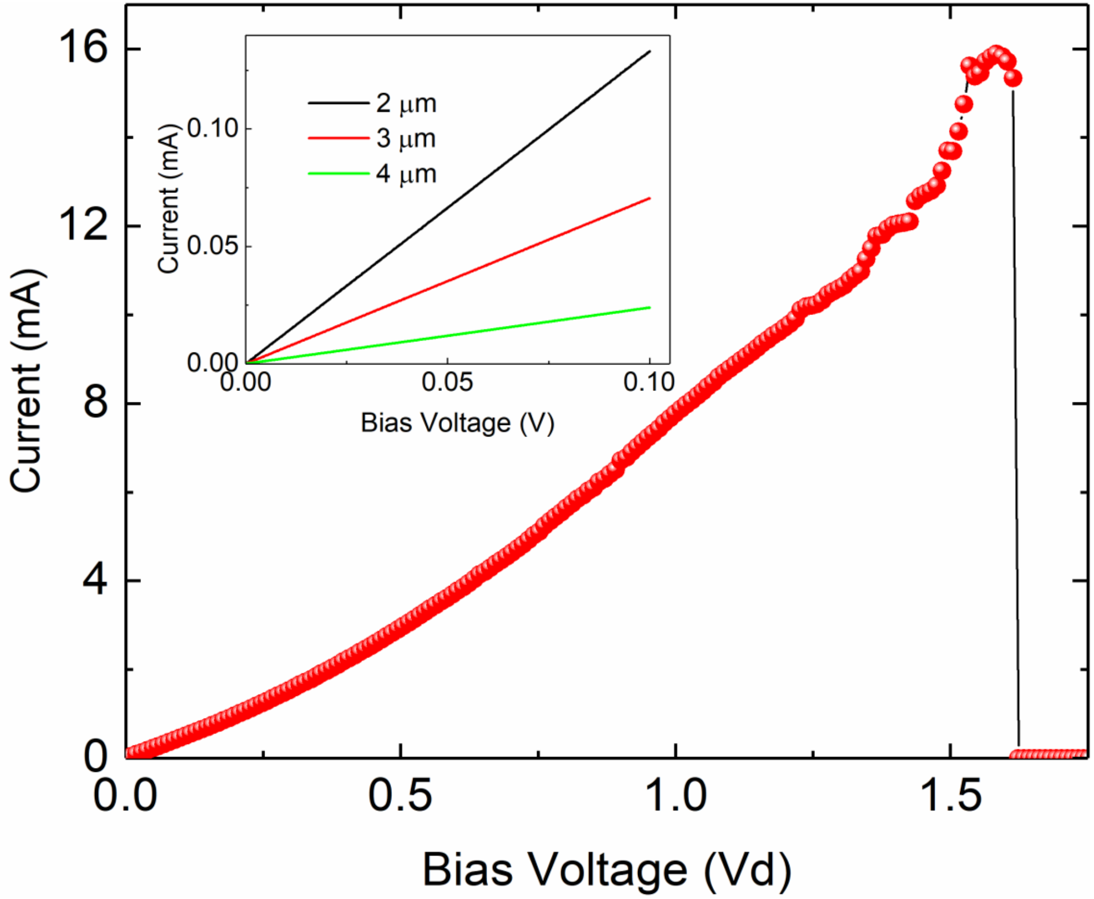
→ High-field I-V characteristics showing the breakdown point. In this specific device the breakdown is gradual.

→ Breakdown current density of about 32 MA/cm^2 — an order-of-magnitude higher than that for copper.

Open question: high currents are sustained in materials with low thermal conductivity

Resistivity is 2.6 – 6.4×10^{-4} Ω-cm.

Current Carrying Capacity of Quasi-1D $ZrTe_3$ van der Waals Nanoribbons

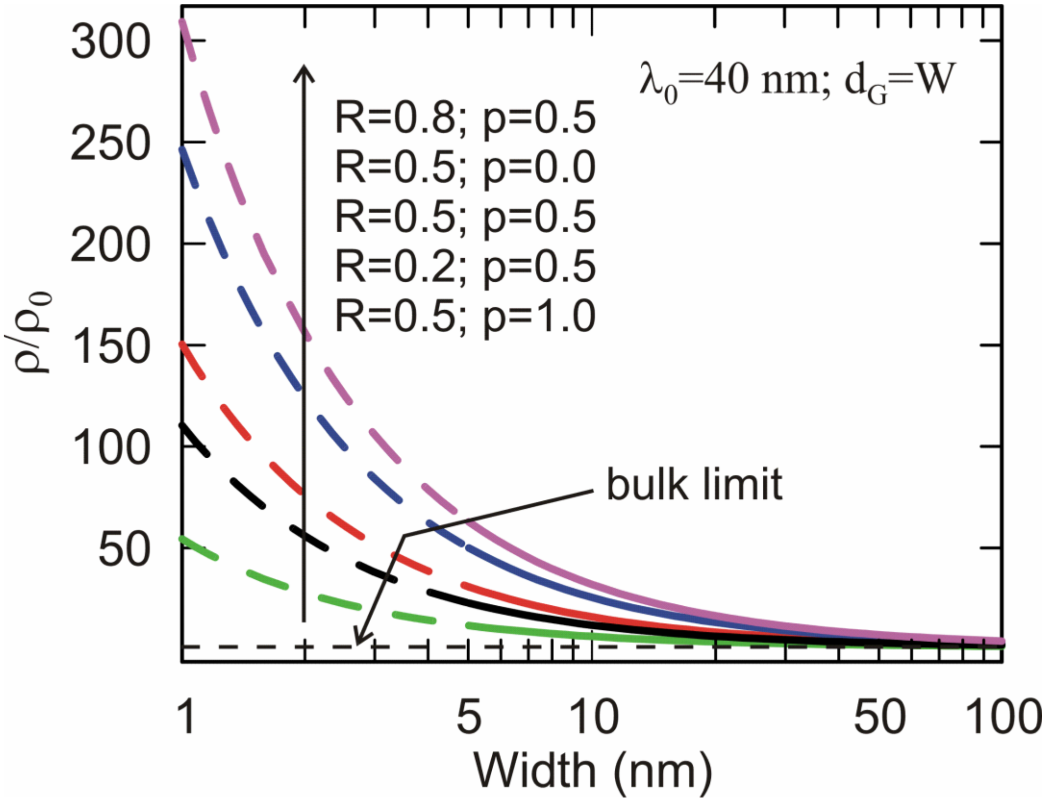


The breakdown current density, calculated with the AFM measured thickness and SEM measured width, corresponds to ~10^8 A/cm^2, reached at the voltage bias of ~1.6 V.

The inset shows low-field I-V characteristics of quasi-1D $ZrTe_3$ devices with different channel lengths.

A. Geremew, et al., "Current carrying capacity of quasi-1D $ZrTe_3$ van der Waals nanoribbons," IEEE Electron Device Lett., 39, 735 (2018).

Comparison with Copper Interconnects – Model Prediction



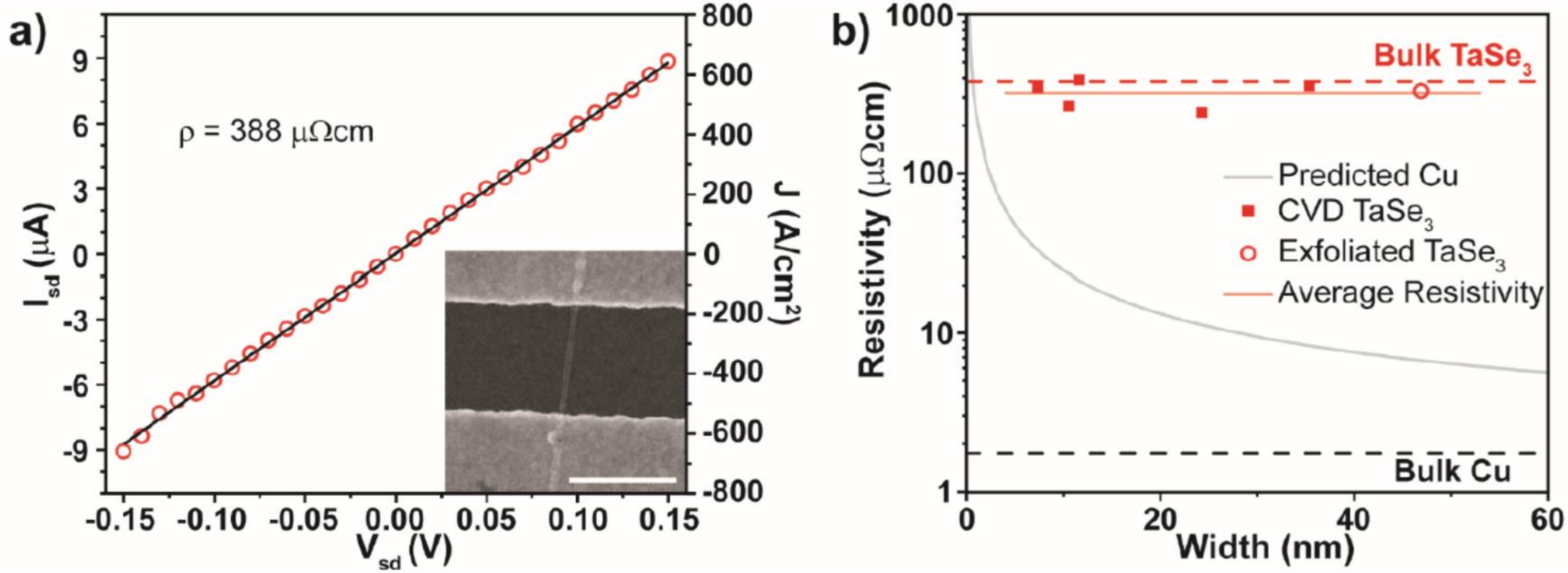
Resistivity trend from the Fuchs-Sondheimer model for the electron–nanowire surface scattering and the Mayadas-Shatzkes model for the electron–grain boundary scattering.

Electrical resistivity of Cu nanowires normalized to the bulk resistivity as a function of W.

Specularity parameters p defines electron scattering from nanowire surfaces; reflectivity R determines the electron scattering from grain boundaries.

Testing Prototype Interconnects Implemented with CVD Grown Quasi-1D Bundles of $TaSe_3$

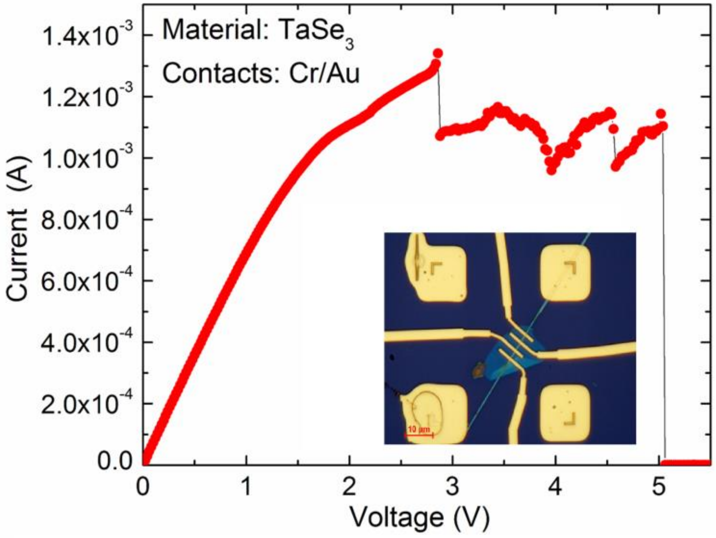
Bartels Group, UCR



A.A. Balandin and L. Bartels, SRC – Intel Corporation: Task 2796.001 Fabrication and Testing of Quasi-1D van der Waals Metal Interconnects

T. A. Empante, et al., “Low resistivity and high breakdown current density of 10 nm diameter van der Waals $TaSe_3$ nanowires by chemical vapor deposition,” Nano Letters 19, 4355 (2019).

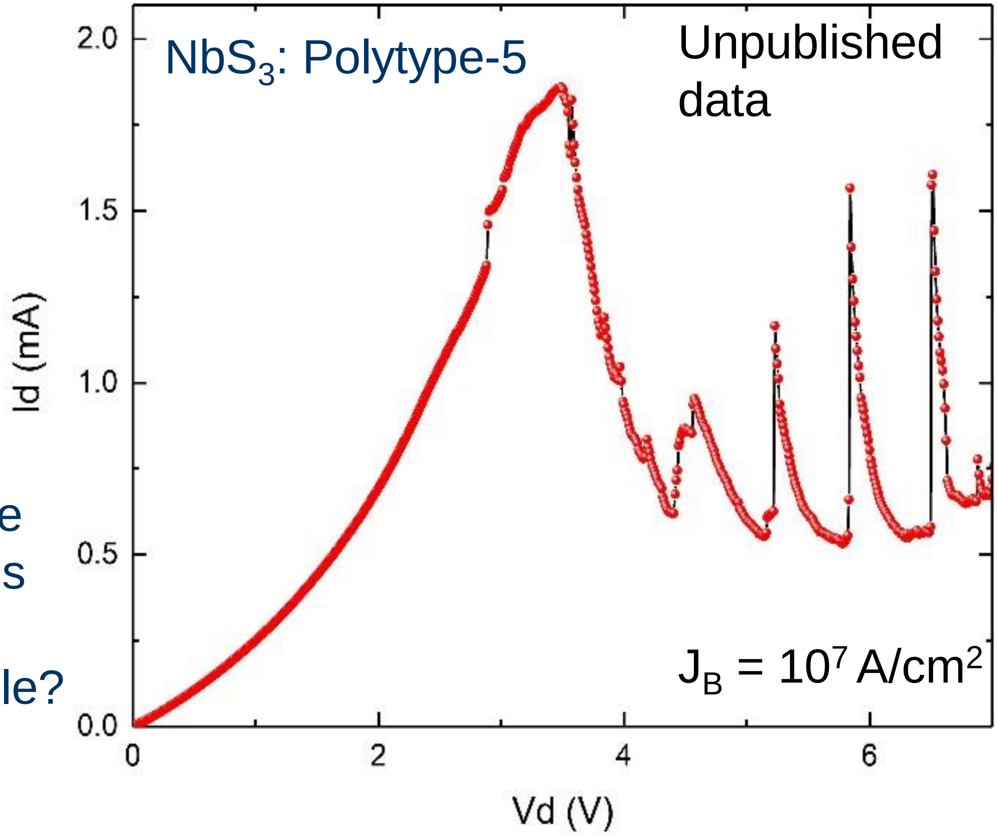
Breakdown in the Bundles of Quasi-1D Materials



→ Step-by-step breakdown in the bundles of the quasi-1D materials

→ Is self-healing function possible?

Unusual Breakdown Behavior



Unpublished data

$J_B = 10^7\ A/cm^2$

Chemical Exfoliation of Bundles of Quasi-1D van der Waals Materials

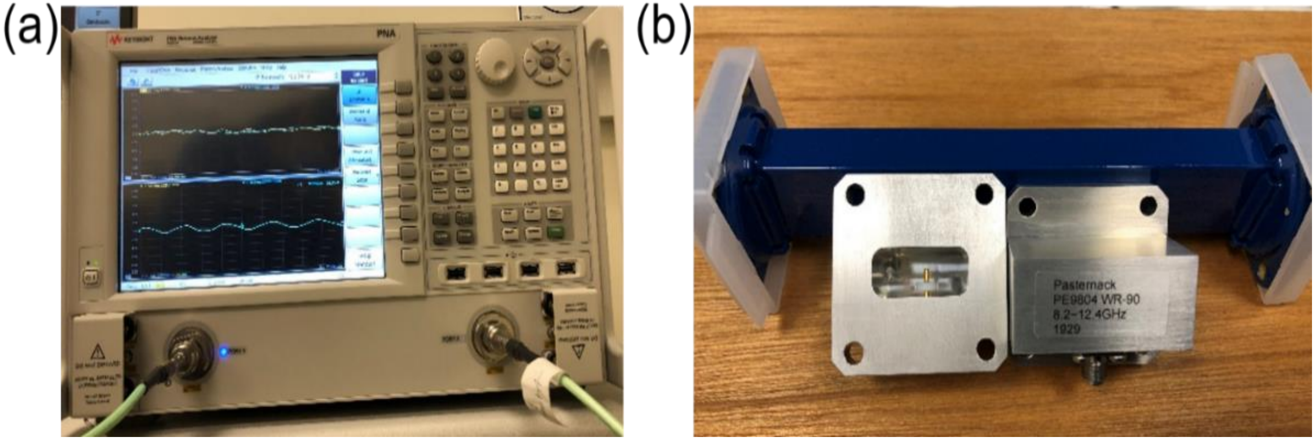
Polymer composite films containing fillers comprised of quasi-1D van der Waals materials.

Fillers can exfoliation into bundles of *atomic threads.*

These nanostructures are characterized by extremely large aspect ratios of up to ~10^6.

Electromagnetic Interference (EMI) Shielding – New Functionality

X-Band frequency range (8.2 GHz – 12.4 GHz)



To determine EMI characteristics, we measured the scattering parameters, S_{ij}, using the two-port PNA system.

Extremely High Frequency (EHF) band (220 GHz – 320 GHz)

EMI shielding efficiency was determined from the measured scattering parameters using Agilent N5245A vector network analyzer (VNA) with a pair of frequency extenders

Z. Barani, F. Kargar, K. Godziszewski, A. Rehman, Y. Yashchyshyn, S. Rumyantsev, G. Cywiński, W. Knap, and A. A. Balandin, “Graphene epoxy-based composites as efficient electromagnetic absorbers in the extremely high-frequency band,” ACS Appl. Mater. Interfaces, 12, 28635 (2020).

EMI Characteristics – Definitions

The scattering parameters define the EM coefficients of reflection, $R = |S_{11}|^2$, and transmission, $T = |S_{21}|^2$,

The coefficient of absorption, A, as $A = 1 - R - T$. A faction of the energy of EM wave, incident on the film, is reflected at the interface.

The effective absorption coefficient, A_{eff}, is defined as $A_{eff} = (1 - R - T)/(1 - R)$.

The total shielding efficiency, SE_T, describes the total attenuation of the incident EM wave by the material of interest.

The shielding parameters can be calculated in terms of R, T, and A_{eff} as follows $SE_R = -10\log(1 - R)$, $SE_A = -10\log(1 - A_{eff})$, and $SE_T = SE_R + SE_A$.

$$SSE = SE_T/\rho \qquad SSE/t = SE/(\rho \times t)$$

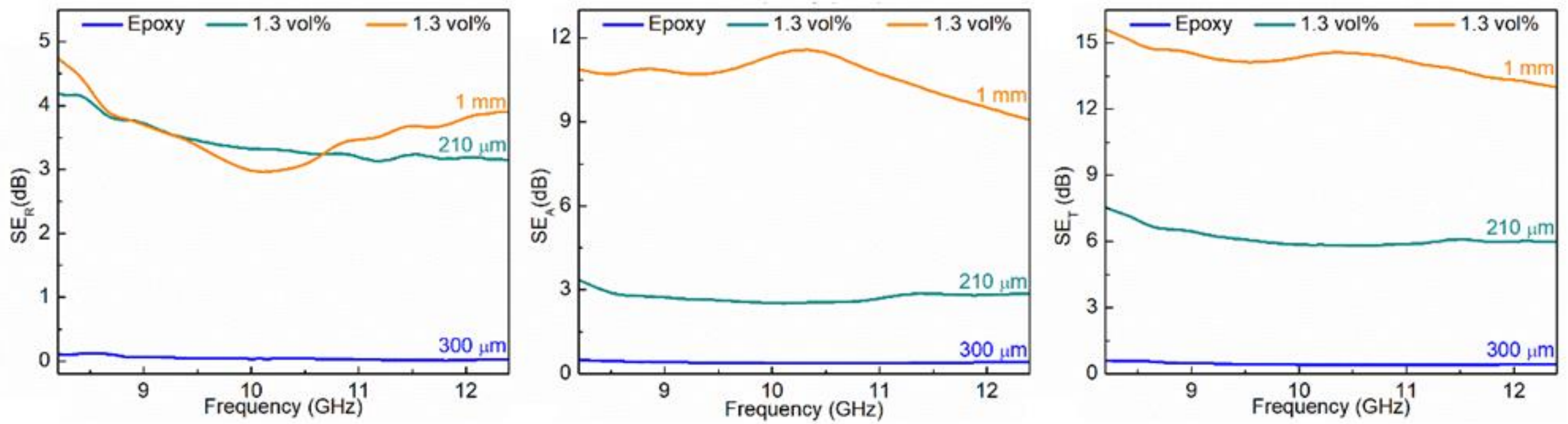
The figure-of-merit $Z_B = SE/(\rho \times t \times m_f)$ where $m_f = M_F/(M_B + M_F)$

$Z_B = SE/(M_F/A)$, here $A = V/t$ is the area

Electromagnetic Interference (EMI) Shielding – New Functionality

X-Band frequency range (8.2 GHz – 12.4 GHz)

Note that only 1.3 vol. % of quasi-1D fillers can provide ~15 dB shielding efficiency, SE_T, in the electrically insulating films (for reference, SE_T=10 dB corresponds to blocking 90% of electromagnetic energy).



Electrically insulating in DC regime

Acknowledgements

Riverside, California, 2019