

Transition from Quasi-2D to Quasi-1D van der Waals Materials:

Electronic Properties of TaSe₃/h-BN Heterostructures

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From Fancy Physics to Practical Applications

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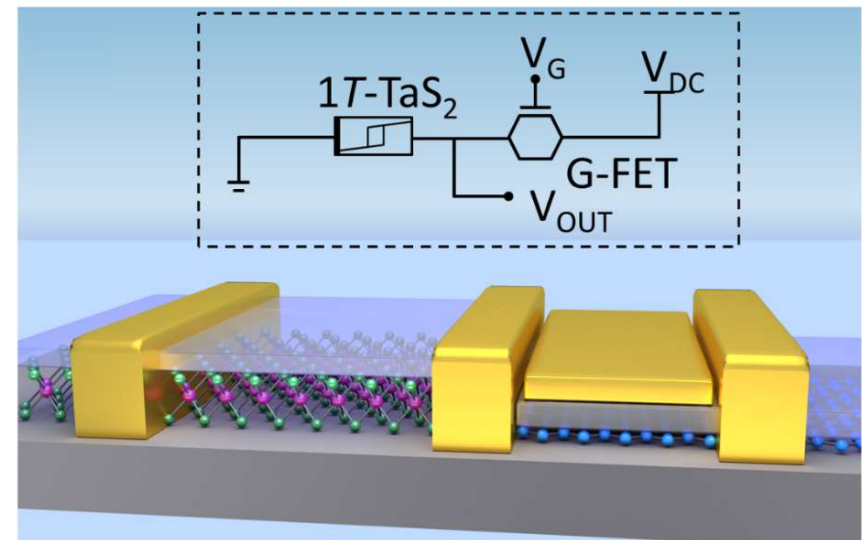
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A charge-density-wave oscillator based on an integrated tantalum disulfide–boron nitride–graphene device operating at room temperature

An Integrated 1T-TaS₂ – h-BN – Graphene Oscillator

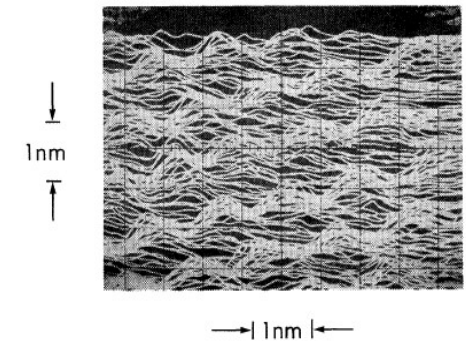
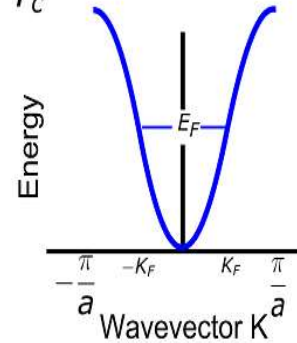
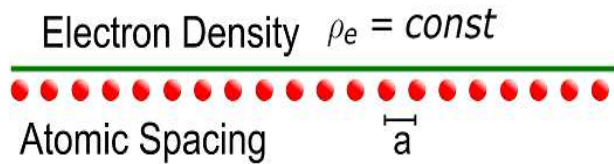
Guanxiong Liu¹, Bishwajit Debnath², Timothy R. Pope³, Tina T. Salguero³, Roger K. Lake² and Alexander A. Balandin^{1*}

The V_{DC} bias is applied at the drain terminal of the G-FET and the V_G bias is connected to the gate terminal of G-FET. Ground is connected to one terminal of 1T-TaS₂ device, while the common terminal of the two devices is the output port.



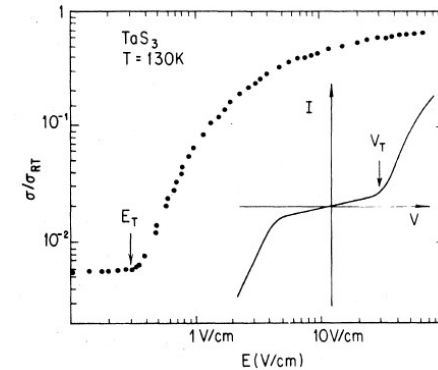
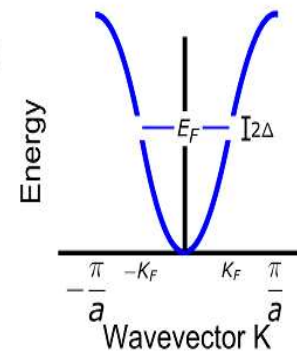
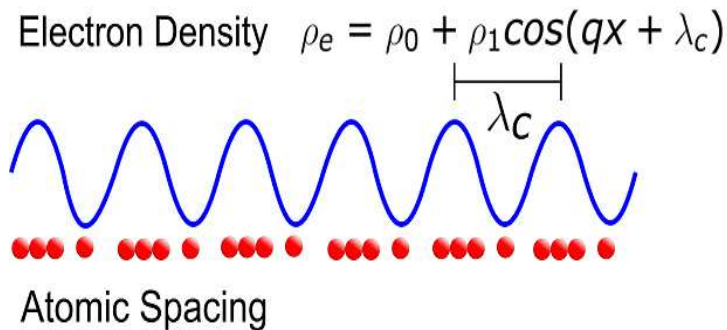
Charge Density Waves: Basics

Normal state $T > T_c$



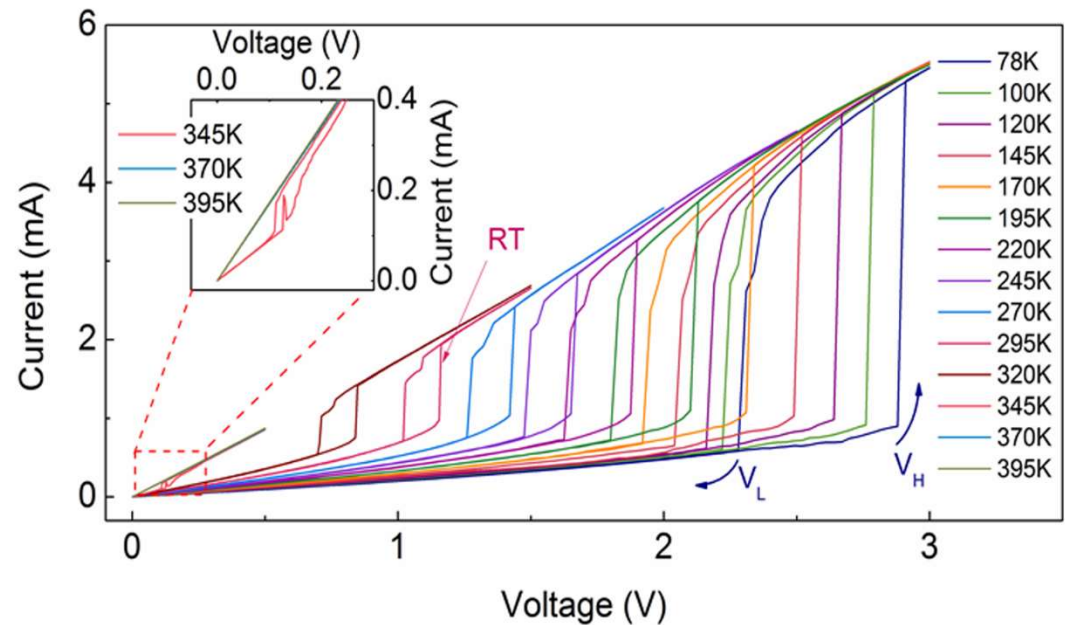
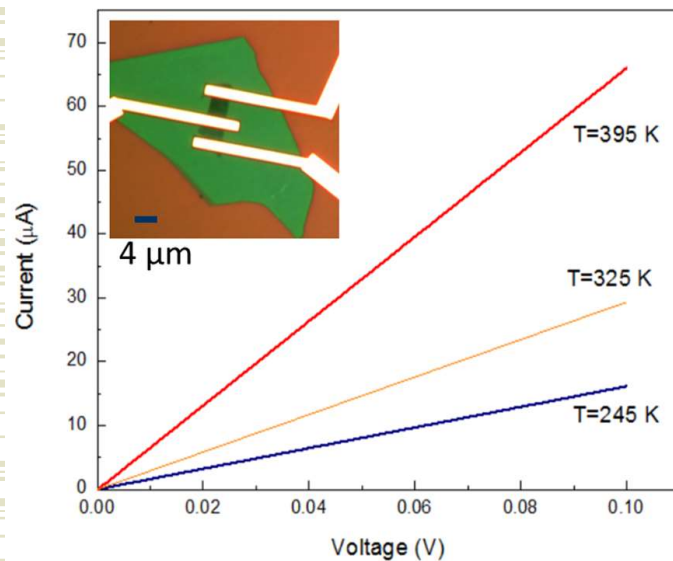
R.V. Coleman, *Phys. Rev. Lett.*, **55**, 394 (1985).

Peierls state $T < T_c$



G. Gruner, *Rev. Mod. Phys.*, **60**, 1129 (1988).

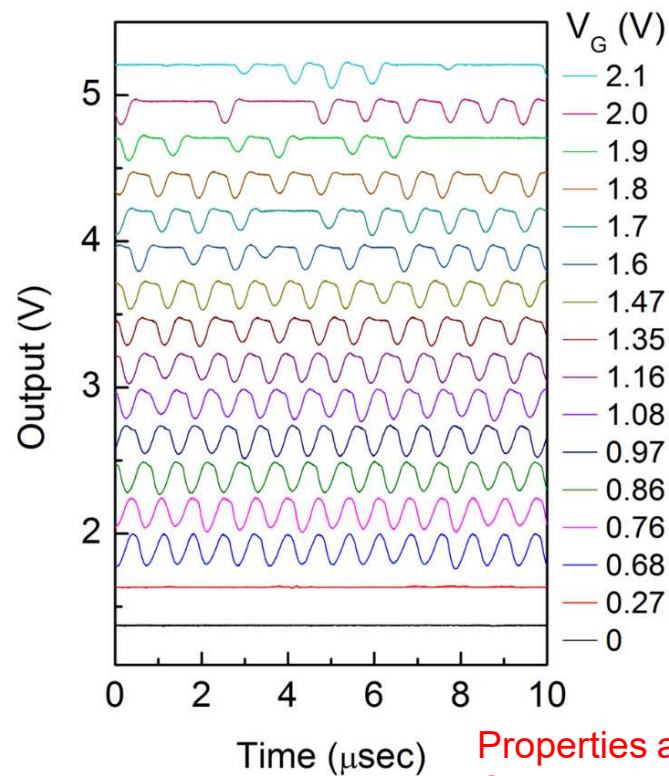
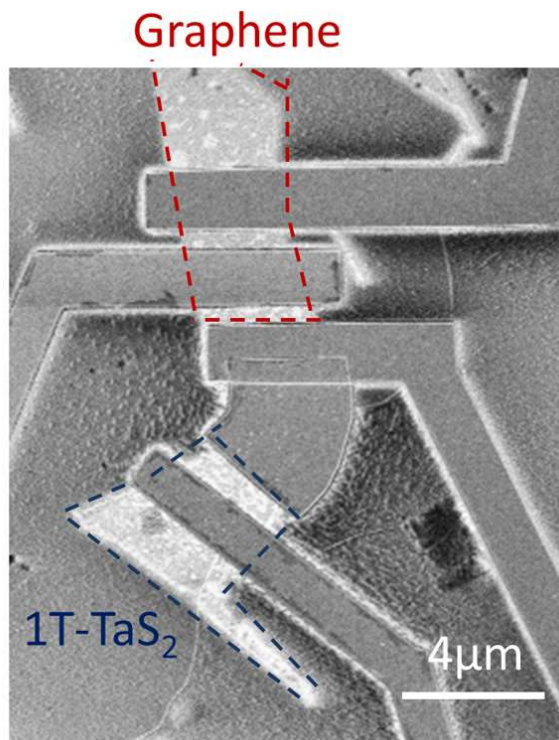
I-V Characteristics of Thin Film 1T-TaS₂



The threshold switching (TS) effect is prominent from 78 K to 320 K. The blue arrows indicate the voltage sweep direction for the measurement at 78 K. For all the other temperatures, V_H is always higher than V_L . The hysteresis window is defined as $V_H - V_L$. The TS is prominent up to 320 K, and becomes less pronounced as the temperature approaches the NC-CDW-IC-CDW transition at 350 K. As shown in the inset, at 345 K (red curve), the TS is still measurable. As T exceeds 350 K, the IV becomes linear.

An Integrated 1T-TaS₂ – h-BN – Graphene Oscillator

The SEM image of the integrated 1T-TaS₂–h-BN–graphene voltage controlled oscillator.



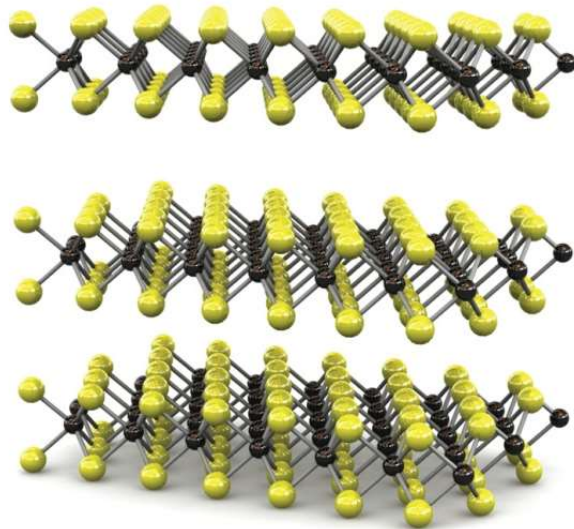
Output waveforms at different gate biases when V_{DC} is fixed at 3.65 V. The oscillation frequency is tunable with gate biases in the range of 0.68 V to 1.8 V. The different waveforms are vertically offset of 0.25 V for clarity.

G. Liu, B. Debnath, T.R. Pope, T.T. Salguero, R.K. Lake and A.A. Balandin, *Nature Nanotech*, 11, 845 (2016).

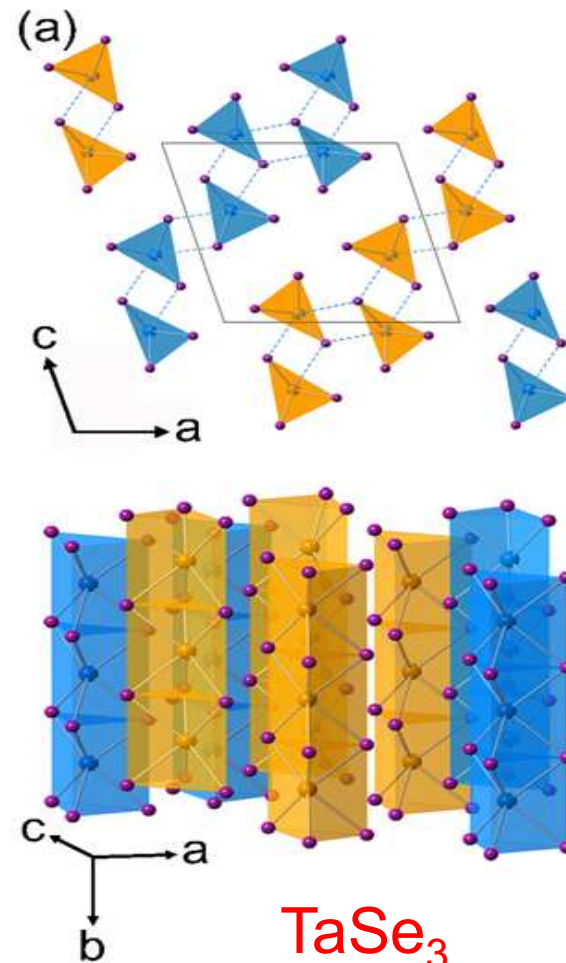
Properties and Device Applications of 2D Charge Density Wave Materials
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Fundamental Science Motivation: From Quasi-2D to Quasi-1D van der Waals Materials

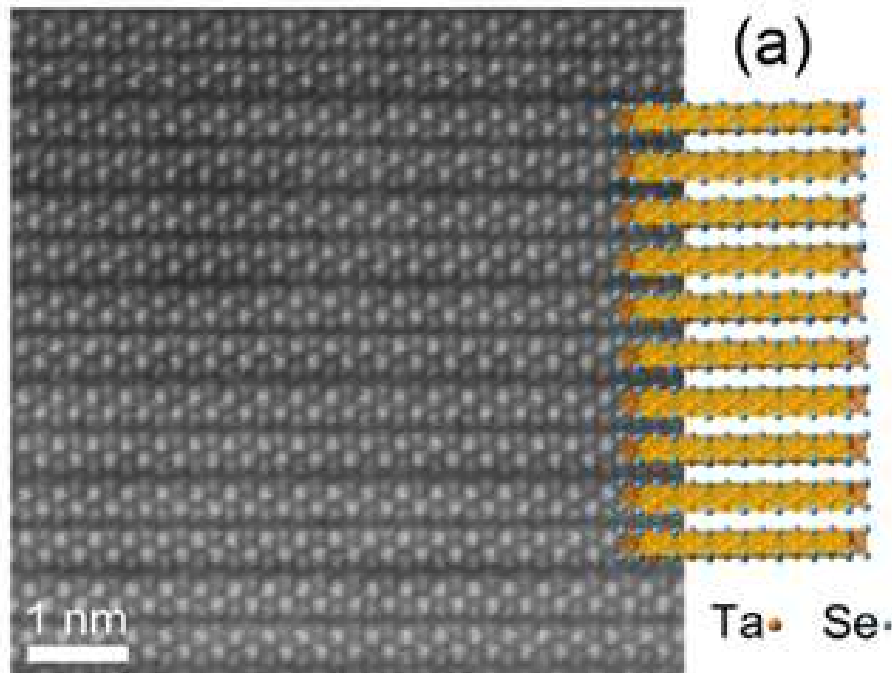
Can we exfoliate Quasi-1D atomic threads like we do quasi-2D atomic planes?



MoS₂



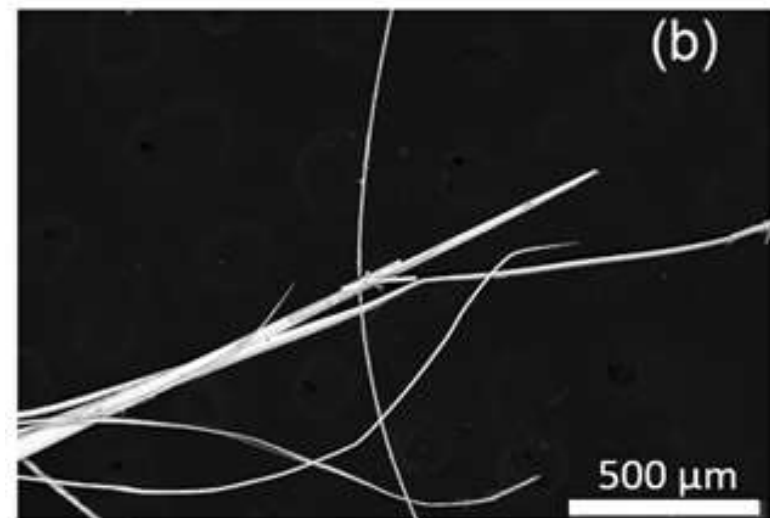
Quasi-1D Crystals Can be Mechanically and Chemically Exfoliated from Bulk TaSe₃



High resolution scanning transmission electron microscopy image of exfoliated TaSe₃ showing pristine metal trichalcogenide chains that extend along the b axis.

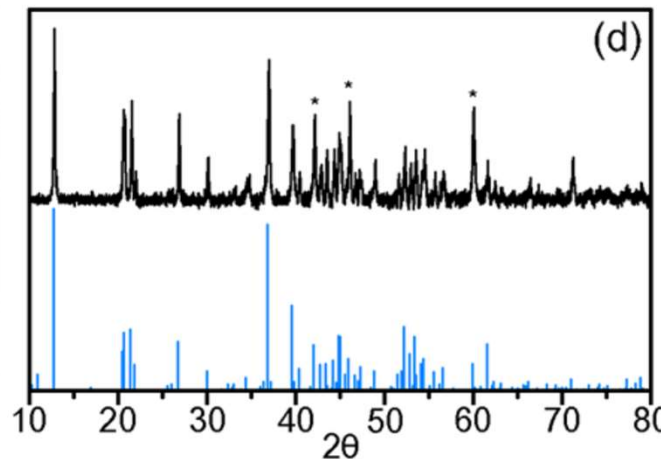
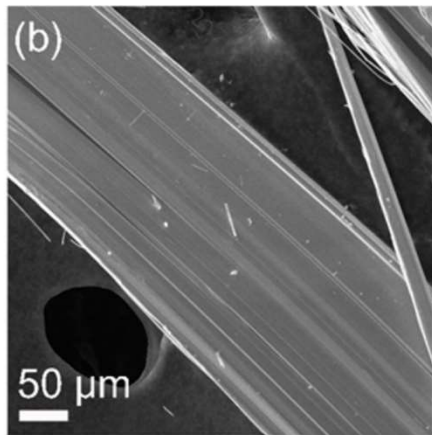
Collaboration:
 Prof. Tina T. Salguero
 University of Georgia

Chemical Vapor Transport (CVT) Method

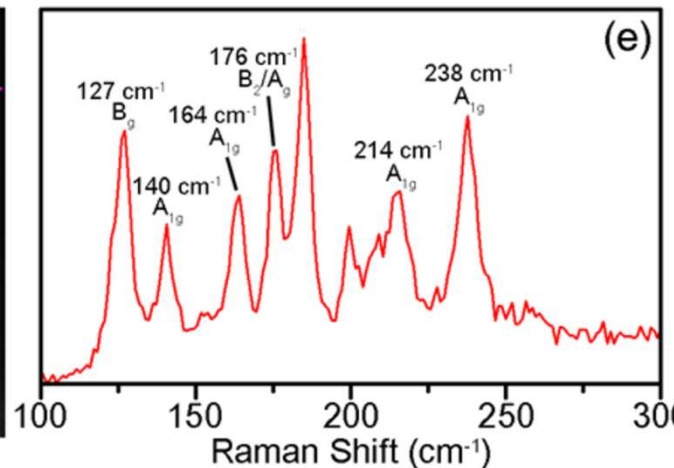
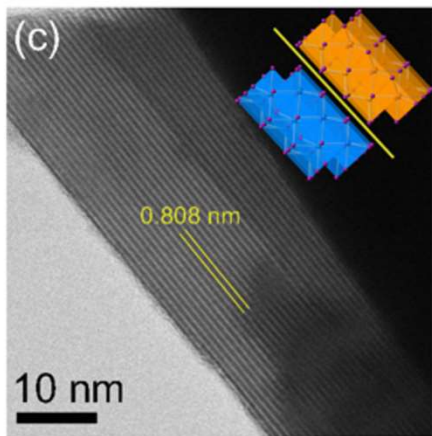


Scanning electron microscopy image of TaSe₃ crystals prepared by CVT method.

Crystallinity of Quasi-1D TaSe₃ Metal

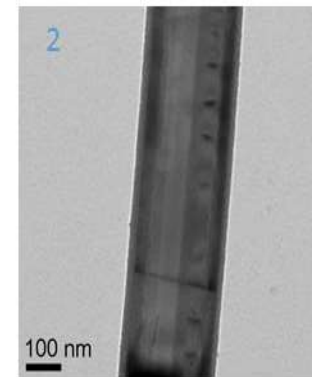
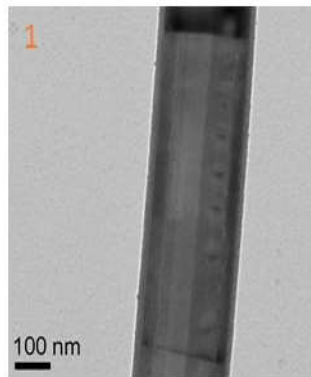
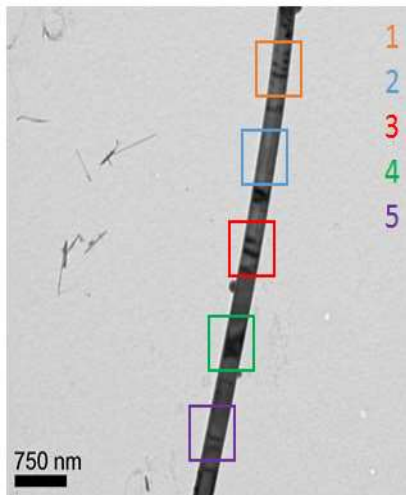


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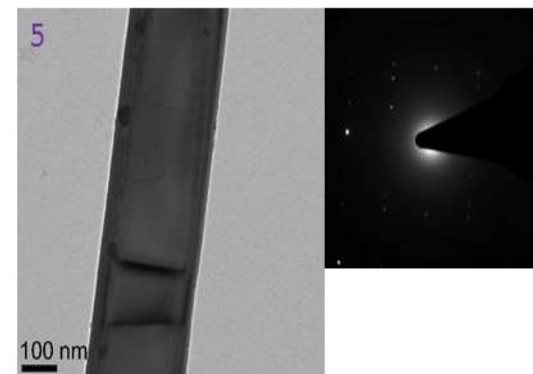
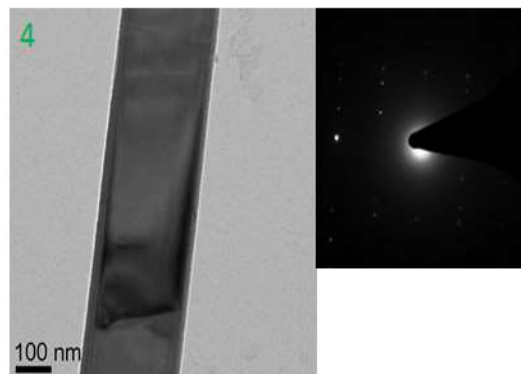
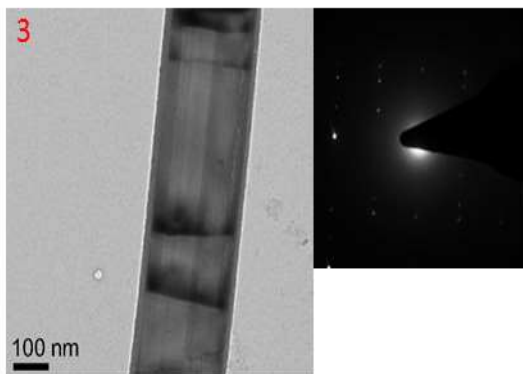


(b) SEM image of a TaSe₃ crystal used in this work. (c) HRTEM image of TaSe₃ after solvent exfoliation. The inset shows the position of the observed (1 0 -1) lattice plane in the van der Waals gap. (d) Powder XRD pattern of TaSe₃ crystals; the experimental data in black matches the reference pattern in blue (JCPDS 04-007-1143). The intensities of peaks marked with * are enhanced due to orientation effects. (e) Raman spectrum of TaSe₃ threads under 633 nm laser excitation.

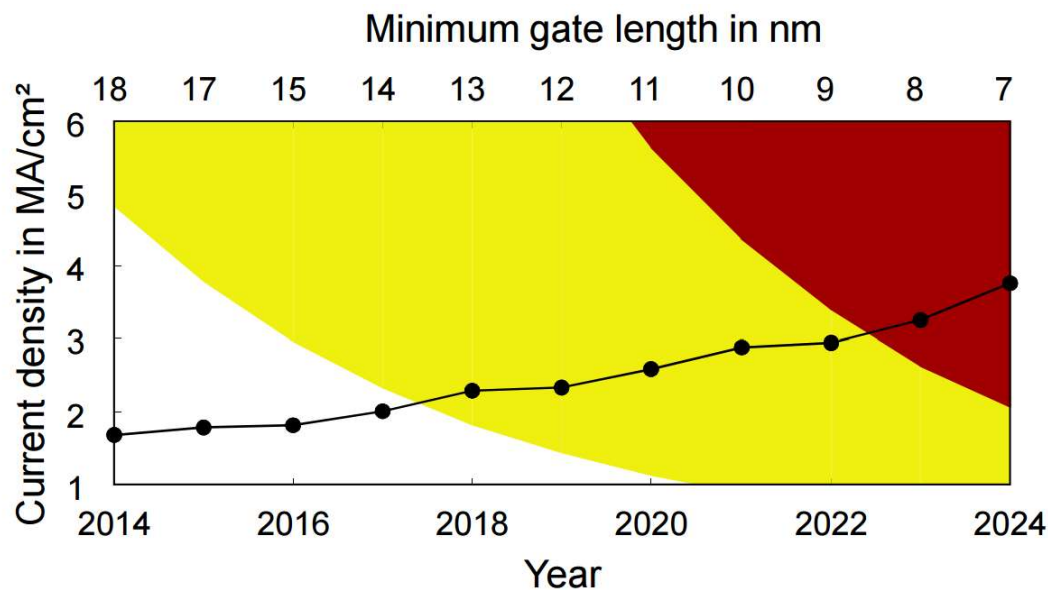
Quasi-1D TaSe₃ Metal van der Waals Nanowires



Selective area electron diffraction data for five various locations along the length of the TaSe₃ nanowires confirming the crystallinity and uniformity of the sample.



Practical Motivations for Quasi-1D Metals: Search of New Interconnect Materials



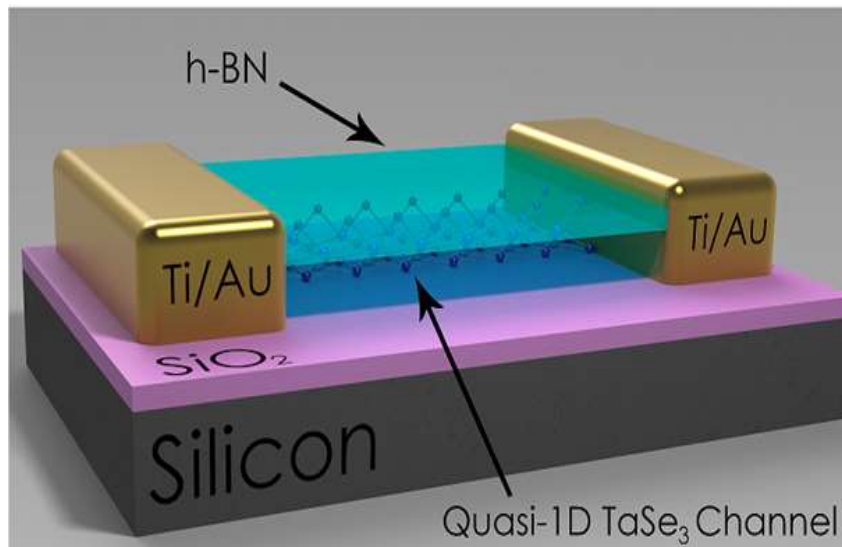
- Currently used manufacturing solutions
- Manufacturable EM-robust solutions are known
- Manufacturable EM-robust solutions are NOT known
- Required current density for driving four inverter gates

According to ITRS:

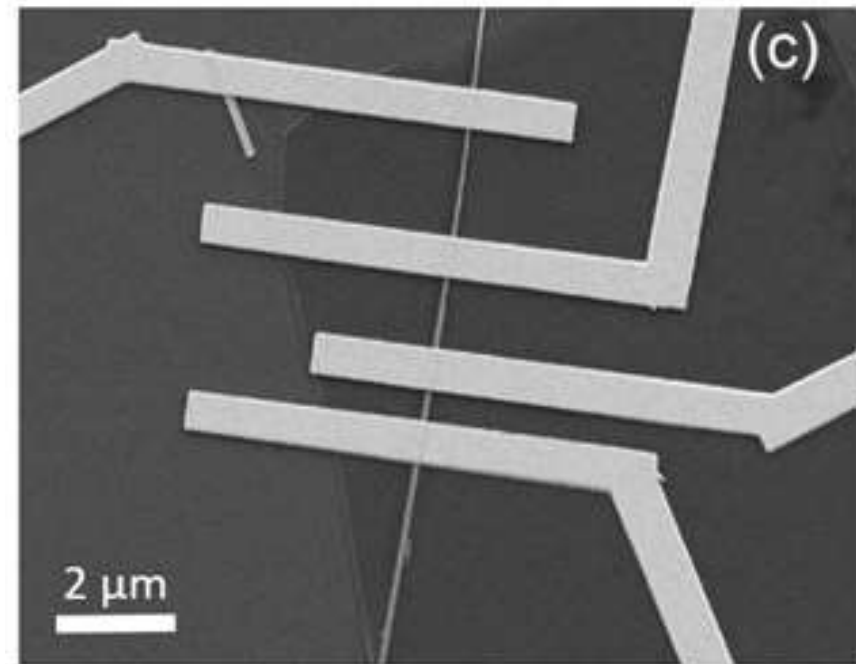
- Current density ~ 1.8 MA/cm² at the half-pitch width of 28.5 nm will increase to ~ 5.35 MA/cm² at the width of 7 nm.
- There is no existing technology with the breakdown current density high enough to sustain such currents.
- The layer thicknesses will decrease from 57.0 nm in 2016 to 15.4 nm by 2028

Boron Nitride Capped Devices with Quasi-1D TaSe₃ Channels

Boron Nitride capping is essential for device fabrication.

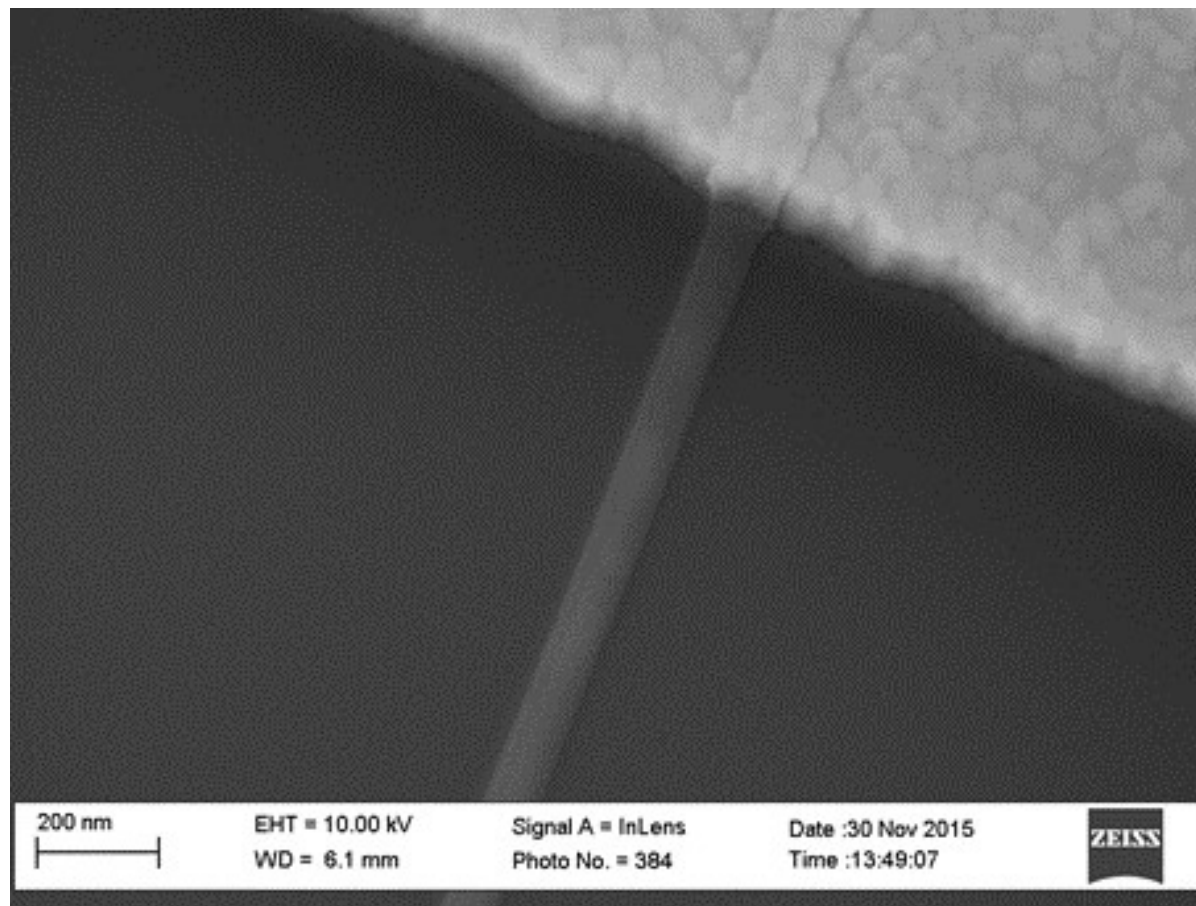


Schematic of the TaSe₃/h-BN quasi-1D / quasi-2D nanowire heterostructures used for the I-V testing.



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

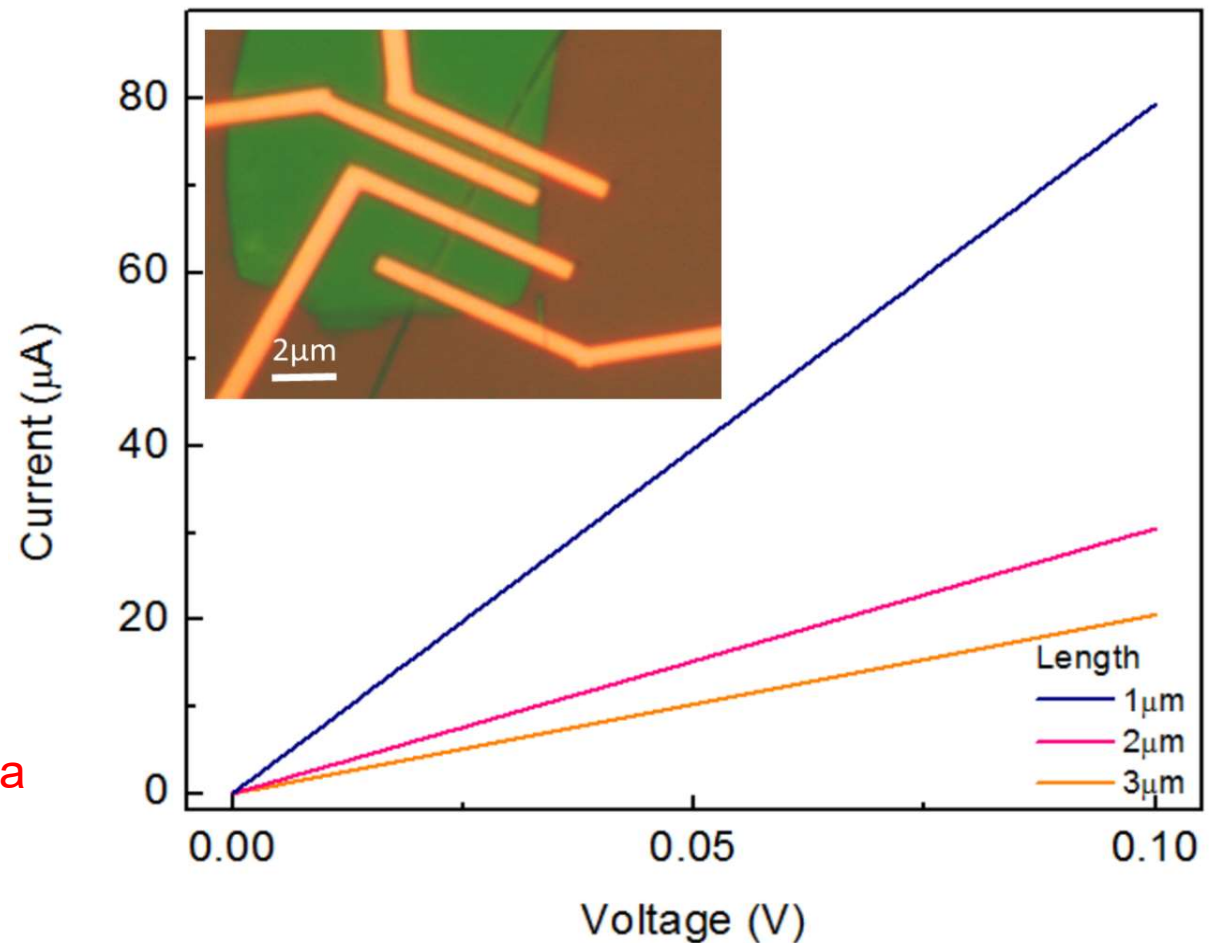
Quasi-1D TaSe₃ Nanowires: Surface Roughness



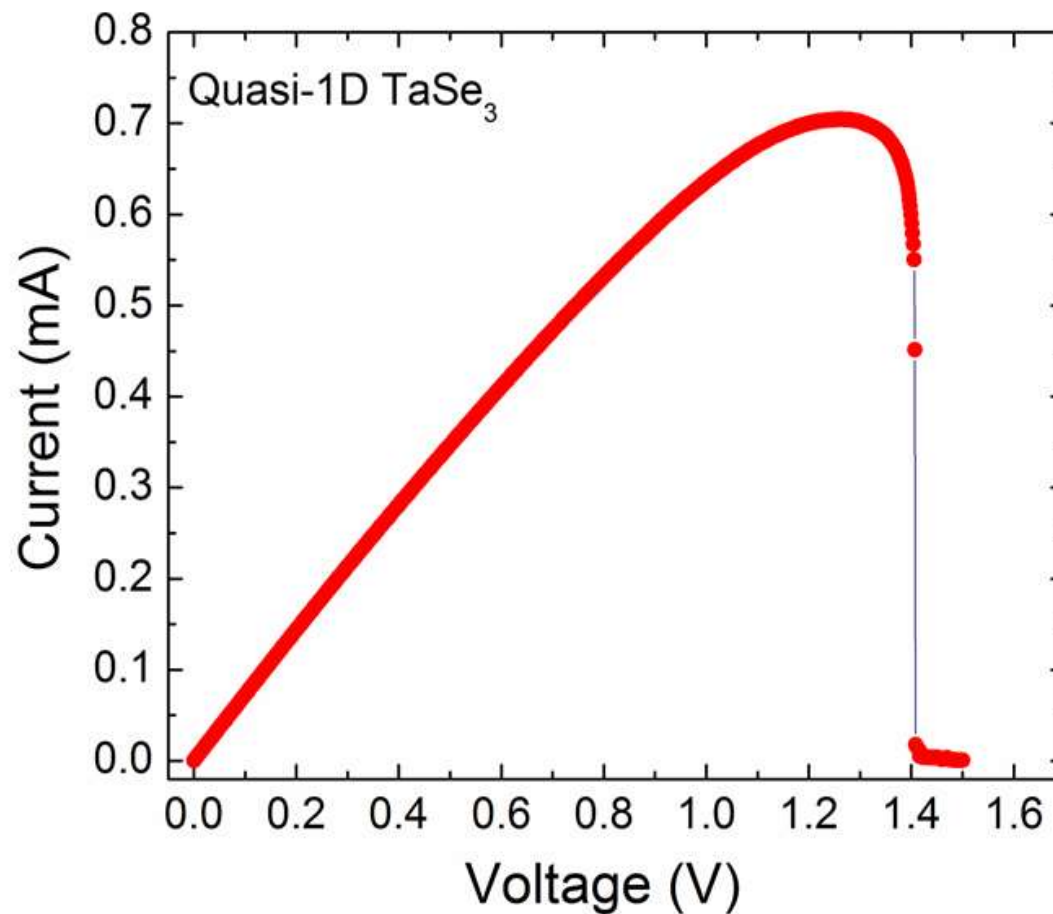
Low-Field Electrical Characteristics of Devices with Quasi-1D TaSe₃ Channels

- Current-voltage characteristics of TaSe₃ devices with different channel length.
- Linear characteristics at low voltage indicates good Ohmic contact of TaSe₃ channel with the metal electrodes.

The contact resistance extracted from TLM data is $2R_C = 22 \Omega\text{-}\mu\text{m}$



Current Density in Quasi-1D TaSe₃ Nanowires

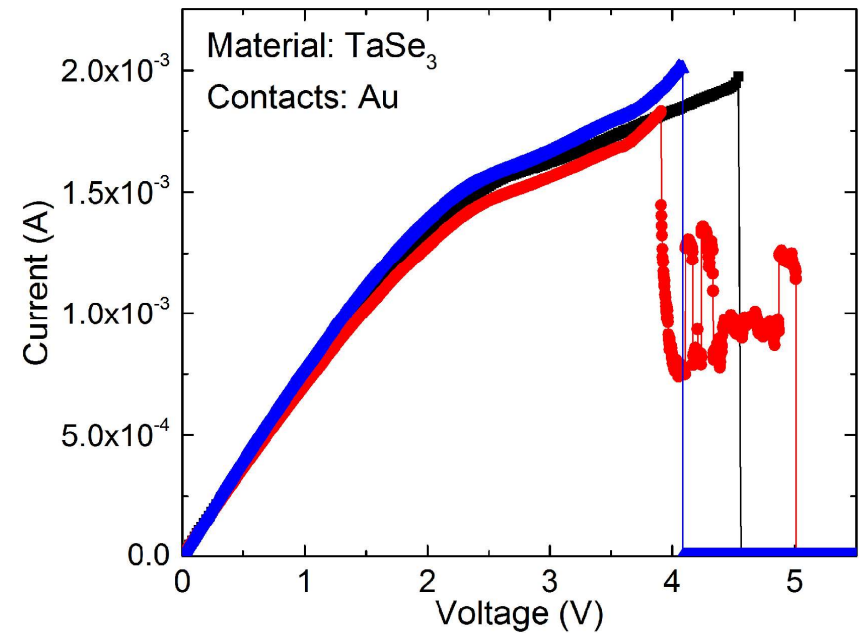
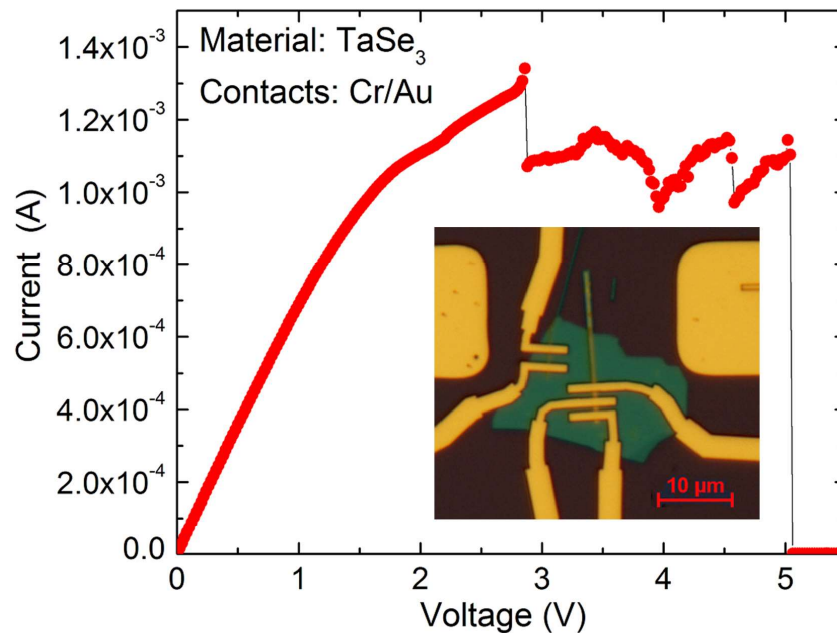


→ High-field I-V characteristics showing the breakdown point. In this specific device the breakdown is gradual.

→ Breakdown current density of about 32 MA/cm² — an order-of-magnitude higher than that for copper.

M.A. Stolyarov, G. Liu, M.A. Bloodgood, E. Aytan, C. Jiang, R. Samnakay, T.T. Salguero, D.L. Nika, S.L. Rummyantsev, M.S. Shur, K.N. Bozhilove and A.A. Balandin, Breakdown current density in h-BN-capped quasi-1D TaSe₃ metallic nanowires: prospects of interconnect applications, *Nanoscale*, **8**, 15774 (2016)

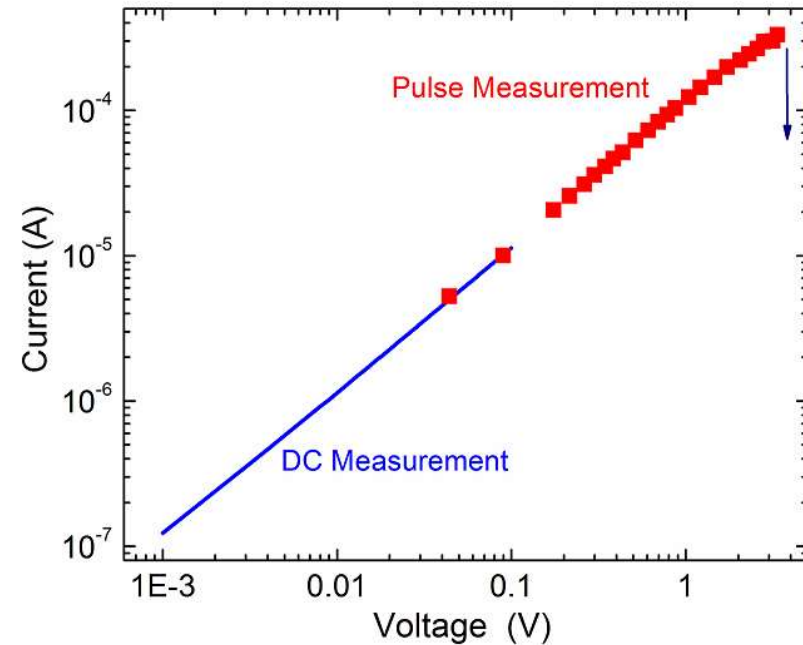
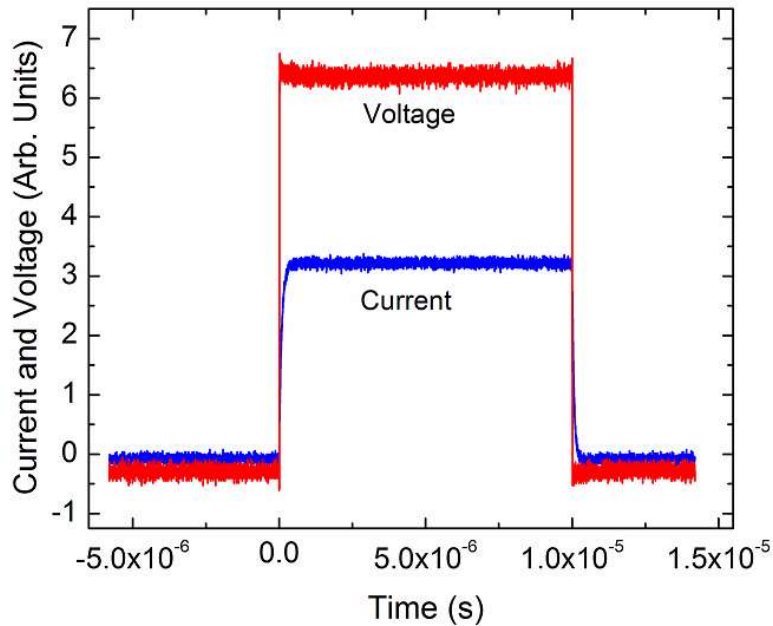
Step-Like Breakdown in Quasi-1D TaSe₃



(a) Current-voltage characteristics of a device with Cr/Au (10/150 nm) contacts. Note a step-like breakdown starting at $J_B = 4 \times 10^6 \text{ A/cm}^2$. (b) Current-voltage characteristics of devices with pure Au contacts (150 nm) showing the step-like breakdowns at $J_B = 6.1 \times 10^6 \text{ A/cm}^2$ (black), $5.7 \times 10^6 \text{ A/cm}^2$ (blue), and $6.3 \times 10^6 \text{ A/cm}^2$ (red).

Pulse Measurements of TaSe₃ Nanowires

Breakdown mechanism: thermal vs. electromigration



Duration and shape of the pulses applied to the h-BN / TaSe₃ nanowire devices (left). I-V characteristics of the devices measured in the pulse and DC regimes (right).

Conclusion: self-heating does not play a major role.

Theory of Electron Transport in Interconnects

The Fuchs-Sondheimer model for the electron–nanowire surface scattering and the Mayadas-Shatzkes model for the electron–grain boundary scattering give the following expression for electrical resistivity:

$$\rho = \rho_0 \cdot \left[2C\lambda_0 \cdot (1-p) \cdot \left(\frac{1}{H} + \frac{1}{W} \right) + \frac{1}{1 - 3\alpha/2 + 3\alpha^2 - 3\alpha^3 \ln(1 + 1/\alpha)} \right]$$

$$\alpha = \lambda_0 \cdot R / (d_G \cdot (1-R))$$

The first term describes the electron scattering on nanowire surface roughness while the second term corresponds to the electron scattering on grains

ρ_0 - bulk electrical resistivity

W - nanowire width

H - nanowire thickness

λ_0 - bulk electron MFP

C = 1.2 – shape factor

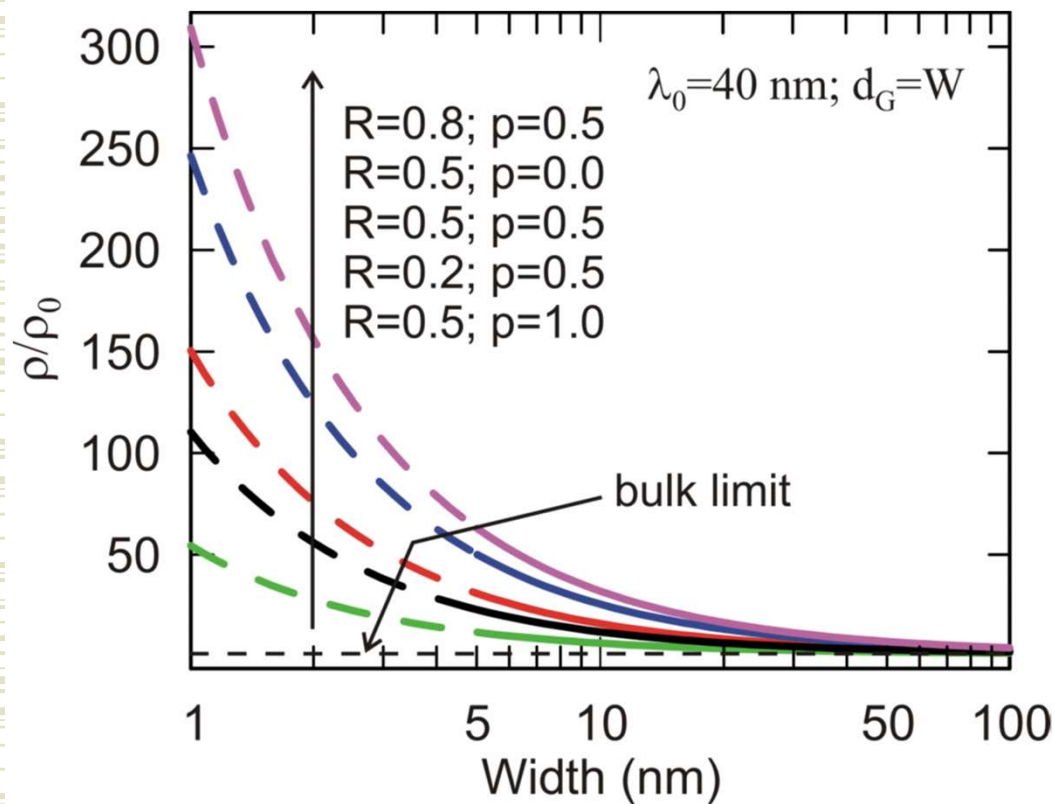
R - reflectivity parameter of the electron – grain boundary scattering

p – specularity parameter for electron – surface scattering

d_G - average grain size

M.A. Stolyarov, et al.,
Breakdown current density in
h-BN-capped quasi-1D TaSe₃
metallic nanowires: prospects
of interconnect applications,
Nanoscale, **8**, 15774 (2016)

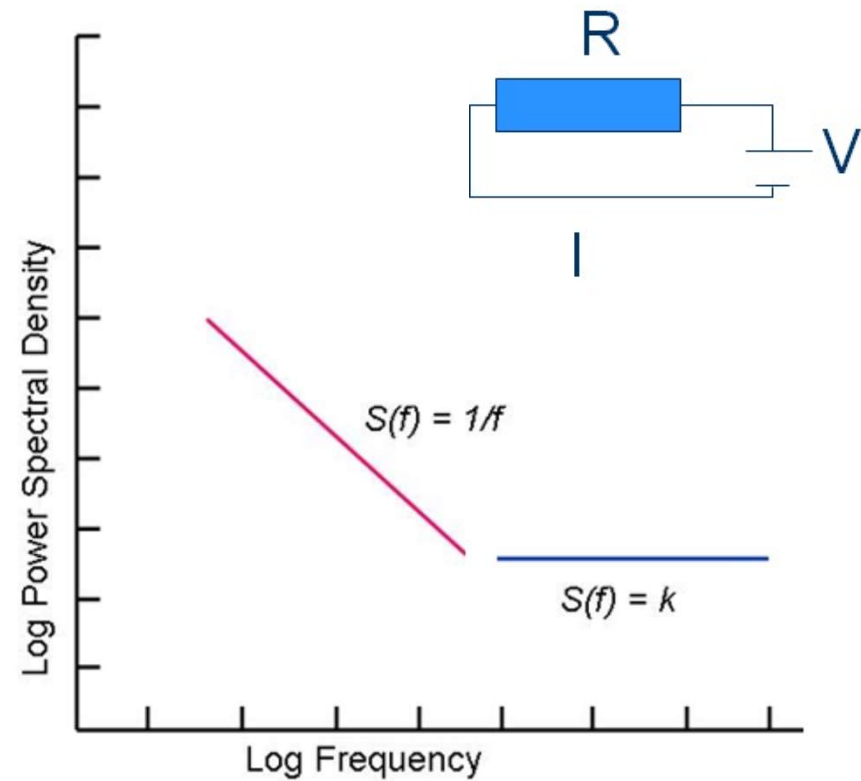
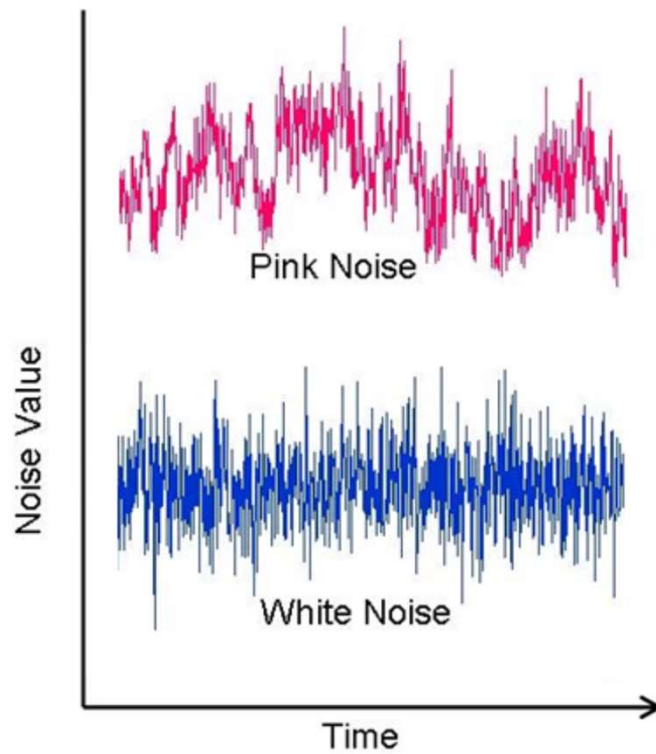
Comparison with Copper Interconnects



Calculated electrical resistivity of Cu nanowires normalized to the bulk Cu resistivity as a function of the nanowire width W . The results are shown for a range of specularity parameters p , which defines electron scattering from nanowire surfaces and parameter R , which determines the electron scattering from grain boundaries.

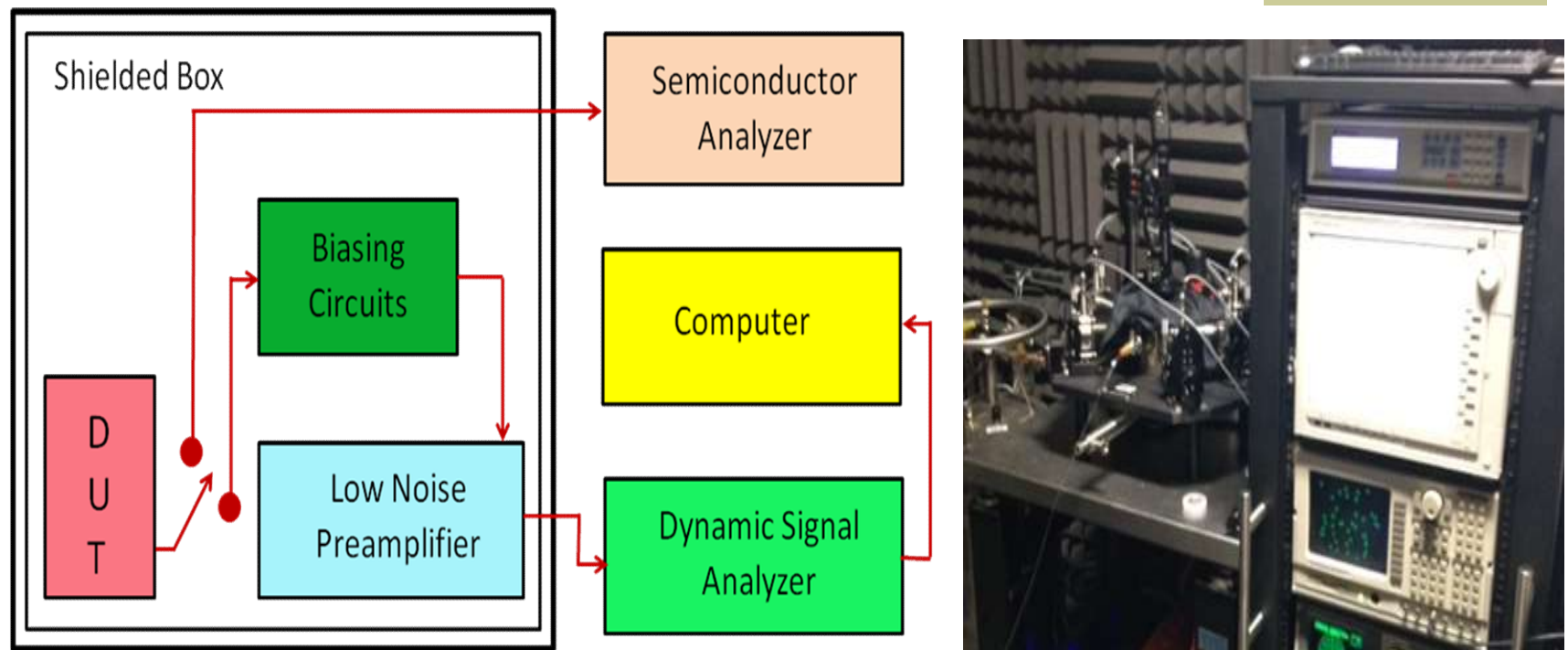
The increase in TaSe₃ resistivity is expected to be less drastic owing to the absence of grain boundaries ($R \rightarrow 0$) and smoother surfaces ($p \rightarrow 1$).

Low-Frequency Flicker Noise



Discovered in vacuum tubes - J. B. Johnson, Phys. Rev. 26, 71 (1925). 19

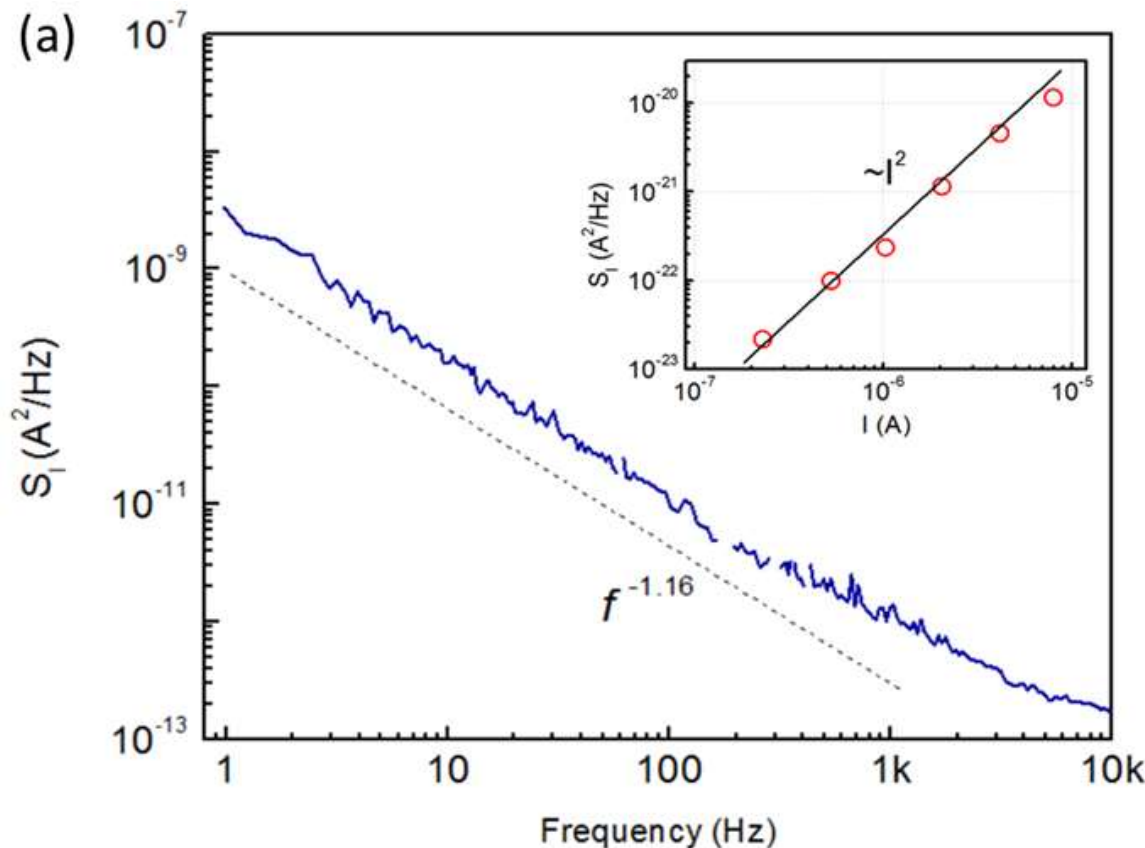
Low-Frequency Noise Measurements



→ The noise measurement set-up is placed inside a special room with the metal and acoustic protection from the environmental noises and electro-magnetic fields

→ Low noise batteries are used for the biasing of the devices

Low-Frequency Noise as Reliability Metric

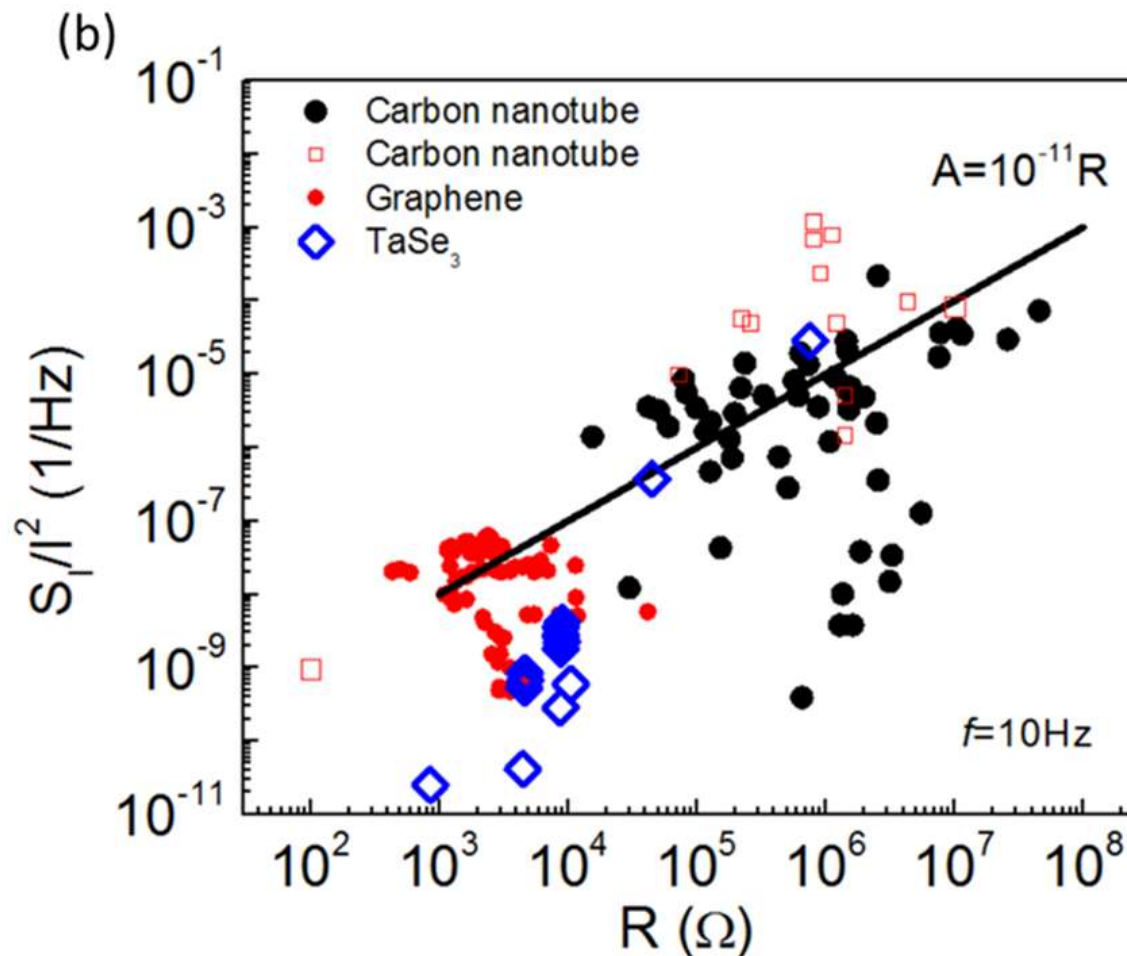


Noise spectrum of TaSe₃ devices at room temperature. The noise spectrum S_1 is flowing $1/f^\gamma$ dependence with $\gamma = 1.1 \sim 1.2$. The inset shows the noise level at $f=10$ Hz as the function of the channel current.

The quadratic dependence of the noise spectrum density S_1 on the channel current I indicates that the $1/f$ noise measured at this current level originates from the TaSe₃ device itself rather than the current induced effects.

G. Liu, S. Rumyantsev, M.A. Bloodgood, T.T. Salguero, M. Shur, and A. A. Balandin, Low-frequency electronic noise in quasi-1D TaSe₃ van der Waals nanowires, Nano Lett., 17, 377 (2017). 21

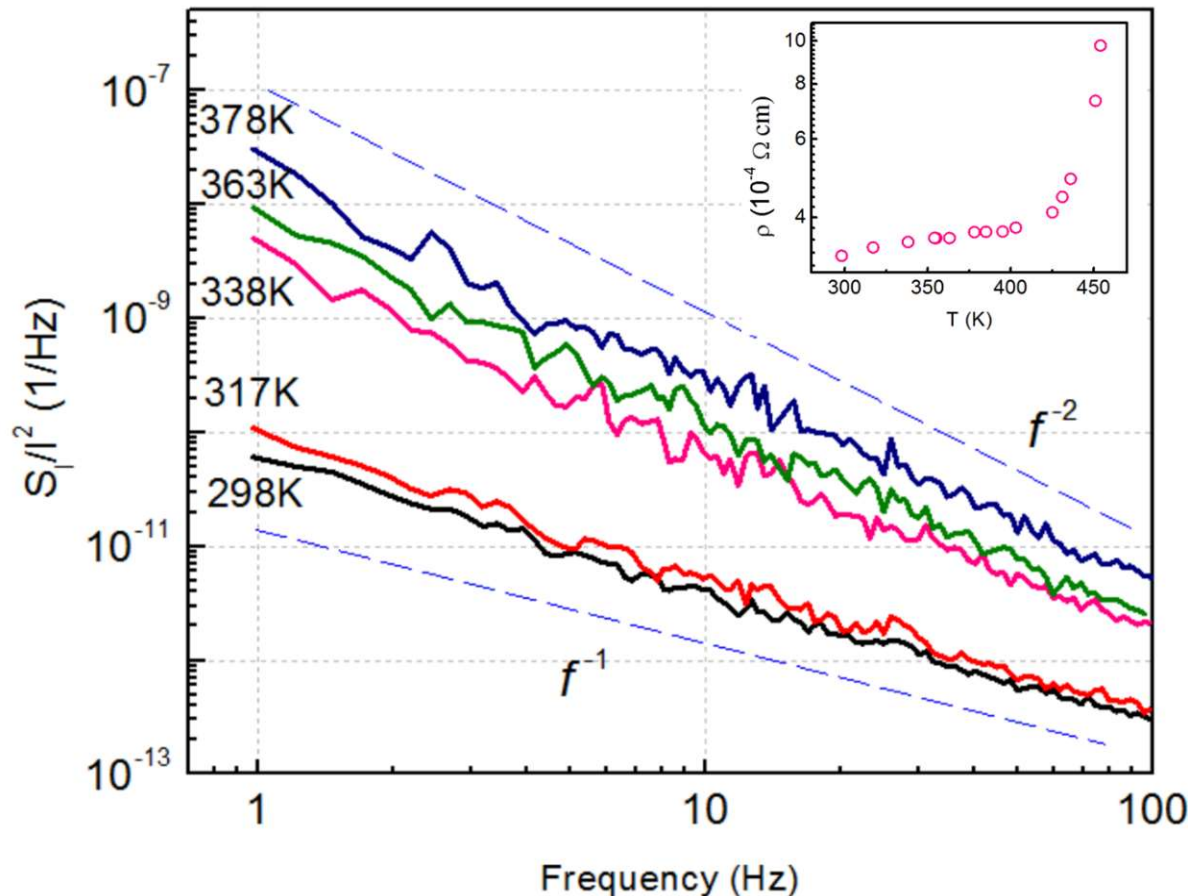
Comparison with Graphene and CNTs



Normalized noise spectrum density as a function of the resistance for different low-dimensional material systems - quasi-1D TaSe₃ nanowires, graphene and carbon nanotubes. For comparison, the empirical relation $A=10^{-11} R$ for the low-frequency noise versus resistance R .

G. Liu, S. Rumyantsev, M.A. Bloodgood, T.T. Salguero, M. Shur, and A. A. Balandin, Low-frequency electronic noise in quasi-1D TaSe₃ van der Waals nanowires, Nano Lett., 17, 377 (2017).

Extracting Electromigration Information from Temperature Dependent Noise Data



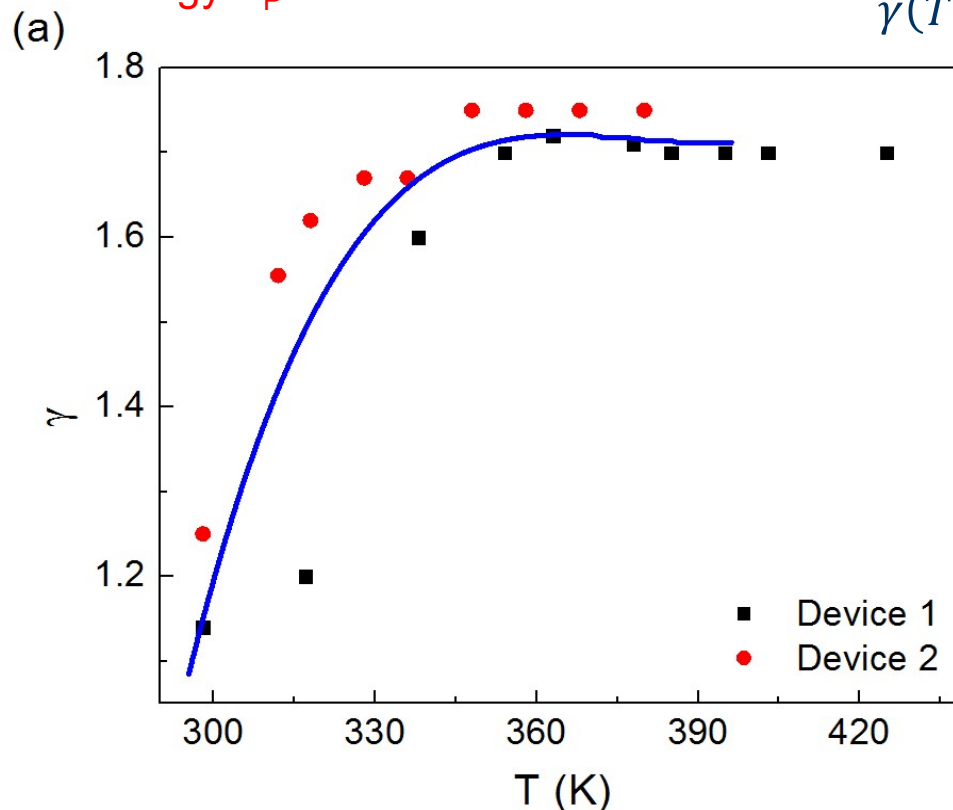
The $1/f$ noise at RT becomes more of $1/f^2$ – type at elevated temperatures. The increased frequency power factor γ suggests the onset of the electromigration processes.

Inset shows the temperature dependent resistance of the quasi-1D TaSe₃ nanowire.

The graduate increase of the resistance with temperature, for $T < 410$ K is typical for metal. The sharply rising resistance for $T > 410$ K indicates the occurrence of electromigration.

Noise Analysis: Dutta–Horn Model

Correlation of the frequency power factor γ with the noise (electromigration) activation energy E_p



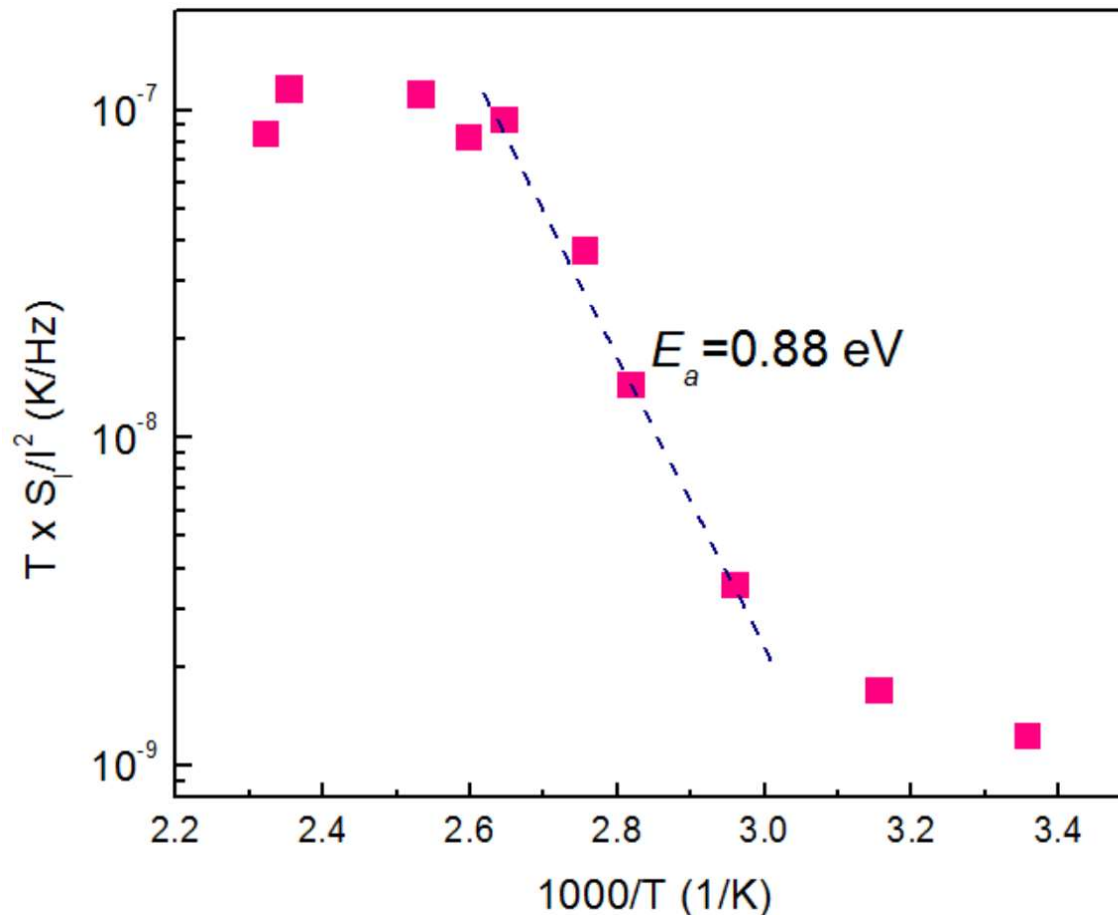
$$\gamma(T) = 1 - \frac{1}{\ln(2\pi f \tau_0)} \left(\frac{\partial \ln S(f, T)}{\partial \ln T} - 1 \right)$$

$$S(f, T) \propto \frac{kT}{2\pi f} D(E)$$

$$E_p = -kT \ln(2\pi f \tau_0)$$

The frequency power factor γ increases from 1.16 - 1.24 at 298 K to 1.72 - 1.75 at 350 K, and remains approximately constant at 1.71-1.75 above 350 K. The blue curve is the fitting of the experimental data.

Noise Analysis: Empirical Model for Interconnects



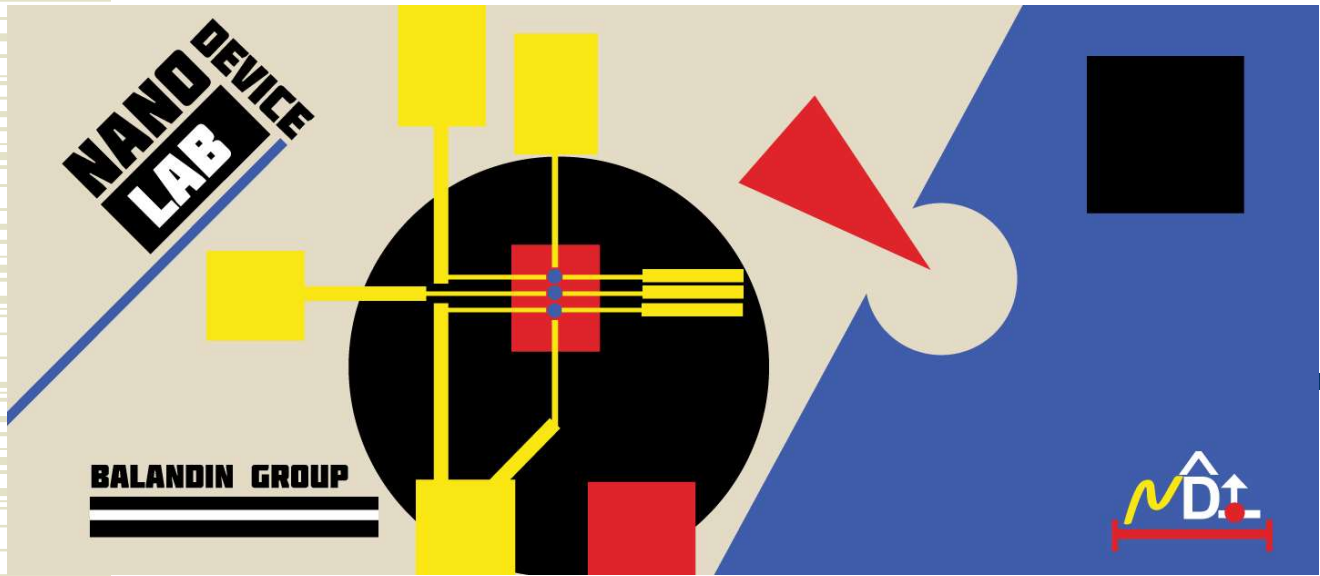
$$S(f) = (Aj^3)/(Tf^\gamma) \exp(-E_A/kT)$$

Temperature dependent 1/f² noise analysis using the Arrhenius plot of $T \times S_1/I^2$ versus $1000/T$. The extracted electromigration activation energy for quasi-1D TaSe₃ nanowire is $E_A = 0.88$ eV.

G. Liu, S. Romyantsev, M.A. Bloodgood, T.T. Salguero, M. Shur, and A. A. Balandin, Low-frequency electronic noise in quasi-1D TaSe₃ van der Waals nanowires, Nano Lett., 17, 377 (2017).

Conclusions

- The concept and approaches of quasi-2D van der Waals materials can be extended to quasi-1D van der Waals materials
- Demonstrated record high 32 MA/cm² current density in a few devices and on average above 10 MA/cm² in numerous devices
- Quasi-1D van der Waals metals allow for ultimate scaling limit – individual atomic thread (1 nm × 1 nm)
- Resistivity scaling in quasi-1D metals can be slower than for conventional metals as the nanowire cross-section decreases
- Breakdown is likely of electromigration nature
- It is possible that other quasi-1D metals may have lower resistivity



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