Electronic Properties and Device Applications of Quasi-2D Charge-Density-Wave Materials

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

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Acknowledging Students

Dr. G. Liu, Apple
Dr. R. Salgado, Intel
Dr. A. Geremew, Intel
Dr. E. Aytan, Intel
Dr. S. Naghibi, Keysight Tech
Dr. F. Kargar, UCR
Z. Barani, UCR
S. Baraghani, UCR

Alexander A. Balandin, University of California - Riverside
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UCR PI: A.A. Balandin

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UCR PI: A.A. Balandin, Co-PI: L. Bartels; Stanford Lead PI: E. Reed

UCR PI: A.A. Balandin, Co-PI: F. Kargar

Alexander A. Balandin, University of California - Riverside
Outline of the Talk

→ Quasi-2D charge-density-wave devices
  → Room temperature operation
  → The use of NC-CDW – IC-CDW transition
  → Switching all the way to metallic phase
  → Noise spectroscopy of phase transitions
→ Radiation hardness
→ Mechanism of switching
→ The search for the “narrow band noise”
→ Conclusions
Charge Density Waves: Bulk 1D Crystals

Normal state $T > T_c$

- Electron Density $\rho_e = \text{const}$
- Atomic Spacing $\frac{1}{a}$

Peierls state $T < T_c$

- Electron Density $\rho_e = \rho_0 + \rho_1 \cos(qx + \lambda_c)$
- Atomic Spacing

Macroscopic quantum phenomena: coherence length $> 1 \mu$m

Quantum materials

Examples of Current Oscillations in Bulk Quasi-1D CDW Materials

Types of CDW Phase Transitions

- There is no uniform mechanism to explain the origin of CDW in different systems, which means truly quantitative predictions of CDW properties for a new material are practically impossible.

- **Type I – CDW in 1D Peierls’ model:** band-gap (or FSN) in electronic structure, Kohn anomaly in phonon spectra, a structural transition in lattice and a metal–insulator transition. **Examples:** NbS$_3$; TaS$_3$

- **Type II – CDW in 2D electron–phonon coupling model:** The CDW in 2D is not driven by FSN. Instead, the CDW phases are dictated by the $q$-dependent electron–phonon coupling (EPC). **Examples:** NbSe$_2$; TaSe$_2$; TaS$_2$

- **Type III – CDW with 3D character:** charge modulation or charge ordering with no indication of FSN or EPC as the driving force. **Examples:** rare earth systems such as $R_5$Ir$_4$Si$_{10}$

Rebirth of the Field of CDW Materials: Quasi-2D Films of 1T-TaS$_2$

Ambient-pressure phases of 1T-TaS$_2$. The phases are: a metallic phase at temperatures above 550 K; an IC-CDW phase above 350 K; an NC-CDW phase above 190 K; a C-CDW Mott phase below 190 K. Also shown are the Ta atom distortions in the fully commensurate phase and the crystal structure of 1T-TaS$_2$.


There are multiple phase transition points – some of them are above RT
The threshold switching effect is prominent from 78 K to 320 K. The blues 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 switching 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 switching is still measurable.

First Room-Temperature CDW Device

Circuit schematic of the oscillator consists of the 1T-TaS$_2$ film, a series connected load resistor, and a lumped capacitance from the output node to ground. The load resistance is 1 kΩ.

Voltage oscillations under different $V_{DC}$. The circuit oscillates when $V_{DC}$ is within the range of 3.83-3.95 V. The frequency is 1.77 MHz, 1.85 MHz, and 2 MHz when $V_{DC}$ is 3.83, 3.86 and 3.95 V, respectively.

Different operation mechanism from early devices – no de-pinning

Allows for high T operation
Integrated $1T$-$\text{TaS}_2$ – h-BN – Graphene VCO

The SEM image of the integrated $1T$-$\text{TaS}_2$–BN–graphene voltage controlled oscillator. The graphene and the $\text{TaS}_2$ are highlighted by dashed lines.

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

1T-TaS$_2$ CDW Devices Under X-Ray Irradiation

TID response of 1T-TaS$_2$ devices up to 1 M rad (SiO$_2$). (a) I-V curves measured after each X-ray irradiation step. (b) Threshold voltages, $V_H$ and $V_L$, threshold currents, $I_H$ and $I_L$ as function of dose. (c) Extracted resistance at the high resistance and low resistance states as a function of dose.

Carrier concentration: $10^{21}$ cm$^{-2}$ - $10^{22}$ cm$^{-2}$

Radiation Hardness of CDW Devices

(a) Circuit schematic diagram of a self-sustaining oscillator implemented with one 1T-TaS$_2$ device and a load resistor.

(b) Oscillation waveform before and after 1 Mrad(SiO$_2$) X-ray irradiation

Proton Bombardment Immune Devices Based on CDW Transition in 1T-TaS$_2$

The quasi-two-dimensional (2D) 1T-TaS$_2$ channels show a remarkable immunity to bombardment with the high-energy 1.8 MeV protons to, at least, the irradiation fluence of $10^{14}$ H$^+$cm$^{-2}$.

Noise Spectroscopy of CDW Phases

IC CDW – Metal Transition in Quasi-2D CDW Materials

Optical image of a representative device (left panel) and a schematic of the device layered structure (right panel). The scale bar is 2 µm.

Resistance as function of temperature for cooling (blue curve) and heating (red curve) cycles conducted at the rate of 2 K per minute.
Noise Spectroscopy of CDW Transitions

- Resistance as a function of the applied electric field measured at RT.
- Noise spectral density as the function of frequency for several values of the electric field, which include the point of transition from the IC-CDW to the normal metallic phase.
- Noise spectral density, measured at f=10 Hz, as the function of the electric field.

Electric Field vs Self-Heating Mechanism in CDW Devices

Summary of electric field induced phase transitions at different temperatures for 1T-TaS$_2$ devices. The variation in the electric field required to include the phase transitions is due to different device geometries, thickness of the layers in the device structures, and other variations in the device designs.

Thermally Driven CDW Switching

Collaboration with Professor J. P. Bird
University at Buffalo

Experimental, and simulated hysteresis window width ($I_c - I_h$) calculated at the constant bias voltage of 1 V as a function of pulse duration. The experimental and theoretical results both follow the same trend, exhibiting a peak at shorter pulse durations and saturating at longer pulse times.

Preliminary conclusion: Modeling shows that the thermally driven device can operate at GHz range.
Current Oscillations in Bulk Quasi-1D CDW Materials

“Narrow band noise” was considered to be a direct evidence of CDW de-pinning and sliding.
The Search for the “Narrow Band Noise” in Quasi-2D CDWs

Noise power spectral density, $S_I$, as a function of the current through $1T$-$TaS_2$ device channel measured at frequency $f=760$ kHz. The red and blue data points correspond to two tested devices.

The lower inset shows the gain, normalized to the gain at $f=30$ kHz, as a function of frequency.

In bulk quasi-1D CDW materials, the linear relationship was explained assuming that $f$ is proportional to the CDW drift velocity, $v_D$, so that $f=v_D/L$, where $L$ is the characteristic distance.

Since $I_{CDW}=neLA$, where $n$ is the charge carrier density, $e$ is the charge of an electron, and $A$ is the cross-sectional area, one obtains:

$$f = \frac{1}{neLA} \times I_{CDW}$$
Have We Found the “Narrow Band Noise” in Quasi-2D CDWs?

Frequency, $f_0$ of the noise peaks as a function of the current through 1T-TaS$_2$ device channel. The inset shows a microscopy image of a representative 1T-TaS$_2$ device structure with several metal contacts.

Relation between the COW current and fundamental oscillation frequency in NbSe$_3$. The inset shows $I_{CDW}/f_0$ vs. temperature. After Bardeen et al. (1982).
The Current Oscillations are due to Hysteresis at the NC-CDW – IC-CDW Transition

I-Vs of tested 1T-TaS$_2$ device which revealed “narrow band noise”. The hysteresis loop at the bias voltage $V = 0.9$ V corresponds to the transition from the NC-CDW phase to the IC-CDW phase induced the applied electric field.


The current oscillations appear to be similar to our earlier result – this is not the “narrow band noise.”

Thank you – Questions?