2D electronic materials for Army applications

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ABSTRACT

The record electronic properties achieved in monolayer graphene and related 2D materials such as molybdenum disulfide and hexagonal boron nitride show promise for revolutionary high-speed and low-power electronic devices. Heterogeneous 2D-stacked materials may create enabling technology for future communication and computation applications to meet soldier requirements. For instance, transparent, flexible and even wearable systems may become feasible. With soldier and squad level electronic power demands increasing, the Army is committed to developing and harnessing graphene-like 2D materials for compact low size-weight-and-power-cost (SWAP-C) systems. This paper will review developments in 2D electronic materials at the Army Research Laboratory over the last five years and discuss directions for future army applications.

Keywords: 2D electronic materials, army applications, size-weight-and-power-cost (SWAP-C), graphene, molybdenum disulfide, hexagonal boron nitride, soldier requirements, flexible electronics

1. INTRODUCTION

In the future, to fight and win in a complex world, soldiers will require new technologies for enhanced situational awareness, command and control, communication, and sensing. New capabilities will rely on increased data processing, computing, and networking-- all carried by the individual soldier. Greater emphasis will be placed on expeditionary forces that are more maneuverable and energy independent. Technologies that are lighter weight, flexible and energy efficient will improve maneuverability by reducing the weight and volume carried by individual soldiers. Energy independence will reduce the logistics footprint. By addressing increased power supply needs, energy harvesting, renewable sources, and improved energy storage density will reduce the logistics burden. Power demand will be reduced through the design and incorporation of novel energy efficient materials combined with conventional electronics, to form heterogeneous, low power electronics.

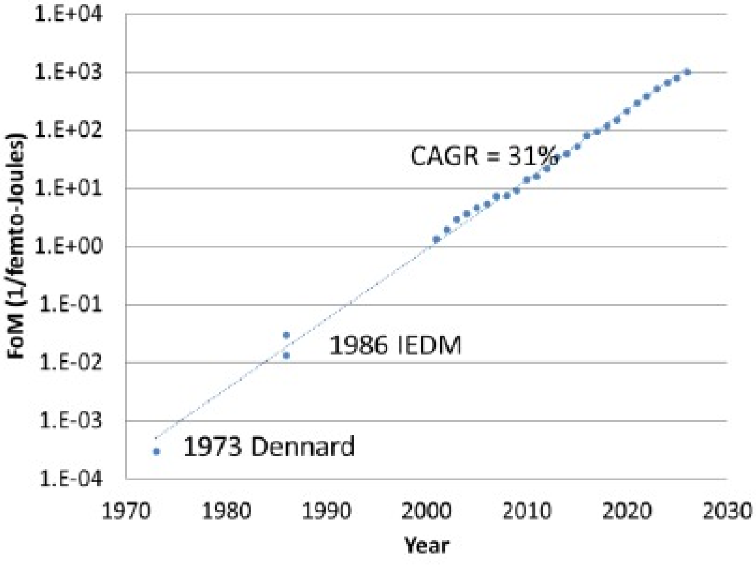

Figure 1. Long term efficiency trend of digital inverters

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As shown in Fig. 1, the scaling of silicon for digital electronics has followed Moore's Law for nearly five decades and has delivered 30% compounded annual growth for the energy efficiency of individual transistors (as defined by the power delay product).[1] Analog devices have piggy-backed on these scaling trends, resulting in the integration of increasingly higher frequency devices and circuits in silicon. For even higher frequency or higher power needs, other semiconductors such as GaAs or GaN are used in place of silicon. Heterogeneous computing aims to integrate semiconductors such as GaN for high-power, high-frequency applications onto silicon.[2] However, fundamental physical limitations are in sight for scaling silicon and related materials which means energy efficiency will plateau, perhaps in the next decade. Further improvements may result from exploiting the novel physics of 2D materials to enable energy-efficient electronic devices and sensors that may be integrated with conventional semiconductors or flexible substrates.

2D materials can be isolated in a few or single atomic layers, and the electronic band structure can be significantly altered depending on layer count, relative orientation between layers, electrics field, and strain. In addition, layering different 2D materials on top of one another we can obtain so-called van der Waals (vdW) heterostructures that have novel electrical, optical and thermal properties. The band structure tunability of 2D materials and the multitude of possible vdW heterostructures offer us new physics and variables to exploit in search of novel energy efficient devices, such as vertical tunneling or spin-based transistors.

With the ultimate goals to extend the predicted energy efficiency plateau of digital and RF electronics as well as to enable flexible electronic applications, we have theoretically and experimentally explored the electrical and thermal properties of single and multilayer molybdenum disulfide (MoS_2) - a 2D material.

2. RESULTS

2.1 Band Structure Engineering

Engineering the band structure, i.e. band gaps and effective masses, using strain is an approach used in silicon technology to increase electron mobility and performance of the subsequent transistor device, which leads to improvements in energy efficiency. In addition, it is imperative to understand how varying strain affects device operation, since flexible devices will operate under various types and magnitudes of strain.

We have utilized Density Functional Theory (DFT) to predict strain-induced variations in electronic properties of MoS_2 bilayer sheets.[3] Our DFT study of bilayer MoS_2 predicted the band gap will shrink significantly for biaxial in-plain strain, whereas compressive strain has less of an effect (see Fig. 2(a)). In addition, as shown in figure 2(b), biaxial strain decreases the conduction band effective mass to a greater degree than uniaxial strain. We show in Fig. 3 how the electron effective mass (m_e) varies compressive and tensile, biaxial and uniaxial strain/stress. Generally the electron mobility increase as is m_e decreased. From Fig. 3, the electron effective mass is reduced by both compressive and tensile/strain/stress, but it is clear that biaxial tensile strain (Fig. 3(a)) yields the lowest m_e. Our DFT study predicts how the band structure of bilayer MoS_2 is modified by strain, and gives insight into how strain could be used to increase the electron mobility, device performance and energy efficiency.

2.2 Temperature-dependent phonon shifts

Raman mapping of 2D materials has become an important tool to characterize layer count, layer orientation, uniformity and many other chemical and electronic material properties. We experimentally measured the in-plane and out-of-plane phonon modes as a function of temperature (see Fig 4(a)) and utilized first-principles molecular dynamics simulations to study the temperature-dependent phonon shifts in monolayer MoS_2 (see fig 4(b)).[4]

Using out combined theoretical and experimental approach, we were able to qualitatively reproduce the temperature-dependent phonon shifts observed with Raman spectroscopy. This has given us some understanding of the temperature-dependent phonon shifts in monolayer MoS_2 and gives insight into the temperature dependence of the electron mobility and the underlying scattering mechanisms that limit energy efficiency.

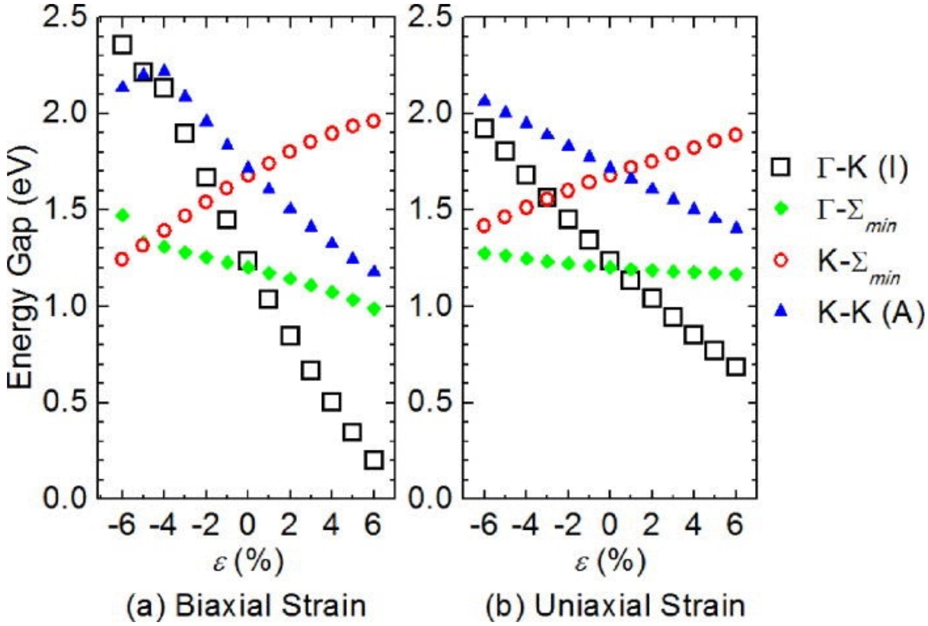

Figure 2. Variations of C–K, C–R$_{\mathrm{min}}$, K–R$_{\mathrm{min}}$, and K–K band gaps with (a) a biaxial strain and (b) a uniaxial strain.[3]

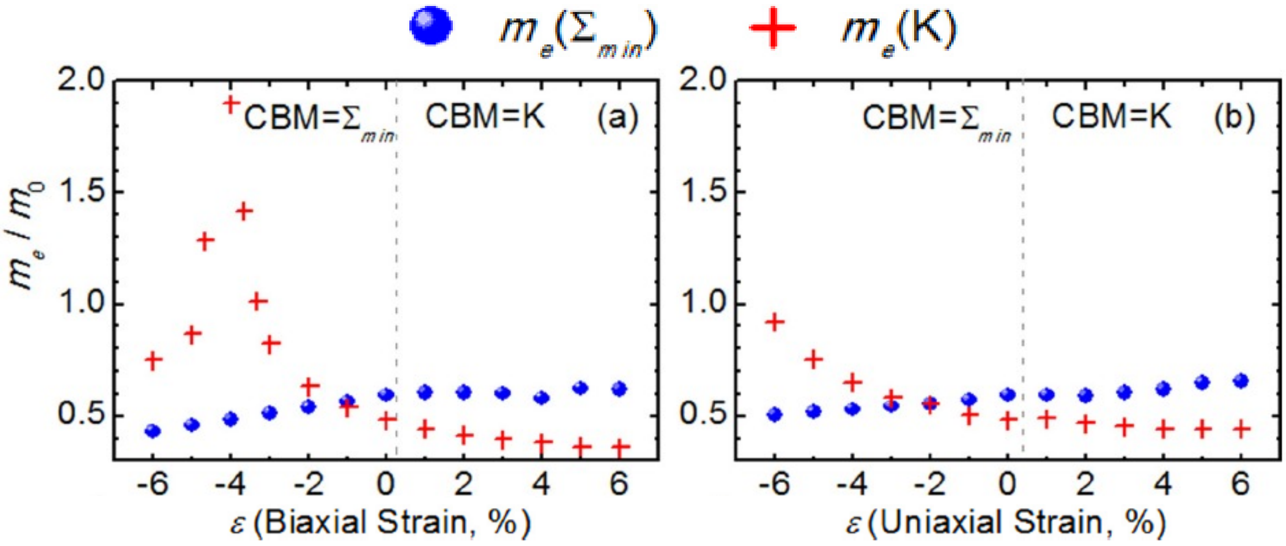

Figure 3. Variations of electron effective mass (m_e) with (a) a biaxial strain and (b) a uniaxial strain.[3]

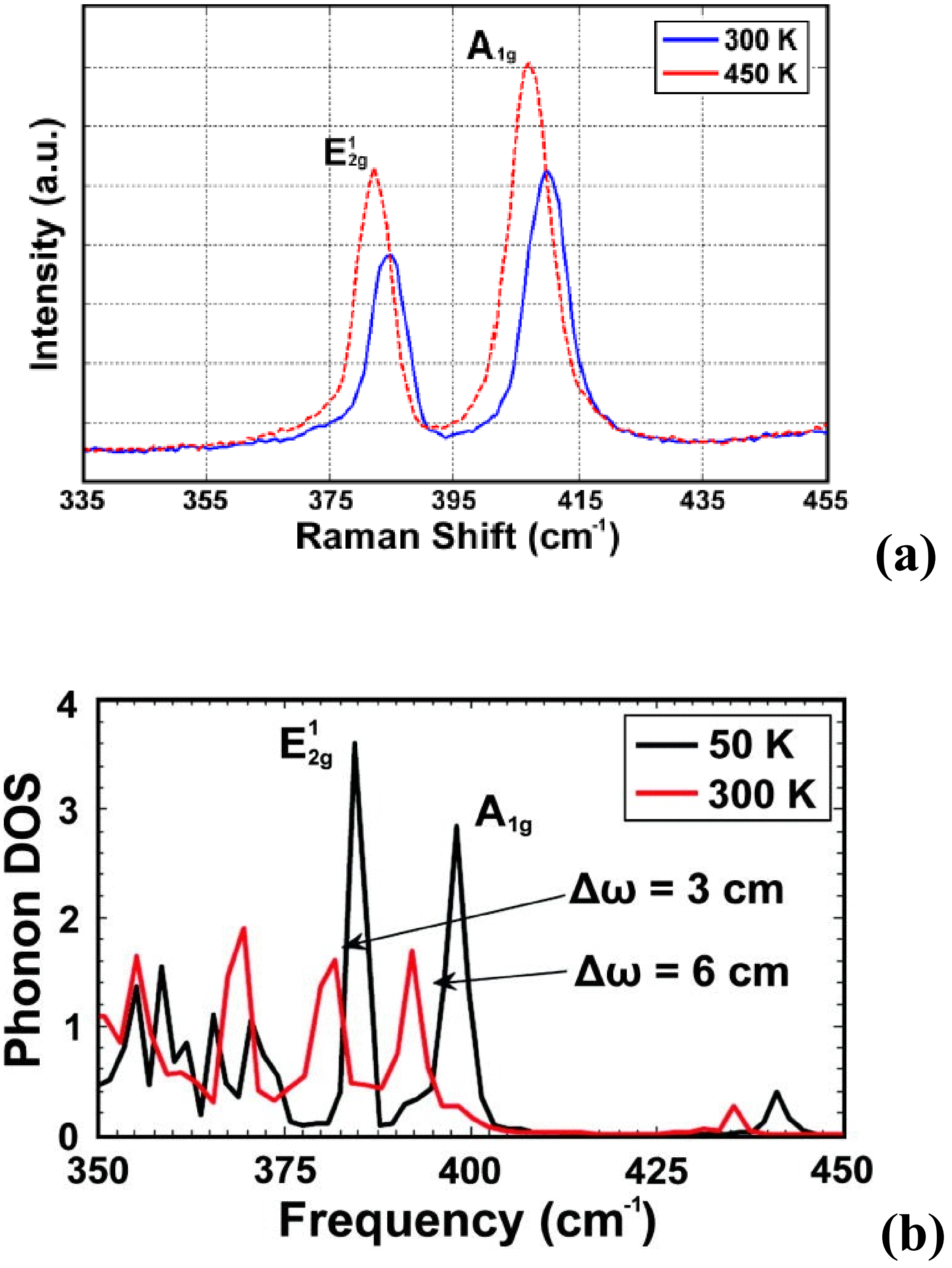

Figure 4. (a) Raman spectra of CVD monolayer MoS2 taken at 300 K and 450 K.[4] (b) The calculated phonon density of states (DOS) for monolayer MoS2 at 50 K and 300 K.[4]

2.3 Materials growth, device Fabrication, and electrical testing

Experimentally we have focused on growing large-area MoS_2 by chemical vapor deposition and fabricating field effect transistors to measure electrical properties, as well as Raman and Photoluminescence mapping to give further insight into material properties.[5]

Specifically, we fabricated field effect transistors in monolayer MoS_2 flakes grown by CVD, measured current–voltage characteristics for various temperatures, and correlated the electrical data to high-resolution Raman maps of the MoS_2 flake. Electrical measurements of fabricated monolayer MoS_2 field effect transistors showed us that the theoretical maximum mobility is difficult to achieve in real-world scenarios. The Atomic force microscopy (AFM), Raman, and Field Emission Scanning electron microscope (FE-SEM) images in Figure 5 show variation in film quality from center-to-edge and contamination between substrate and film. These imperfections in CVD-grown material act as scattering centers that decrease electron mobility and pose challenges to increasing the performance of 2D materials. We show in Fig. 6 the hysteresis we observed in the output characteristics of the field effect transistor. We explained the hysteresis model with a multi-level charge trap model which further demonstrates the complexity of integrating 2D materials into energy efficient electronic circuits.[6]

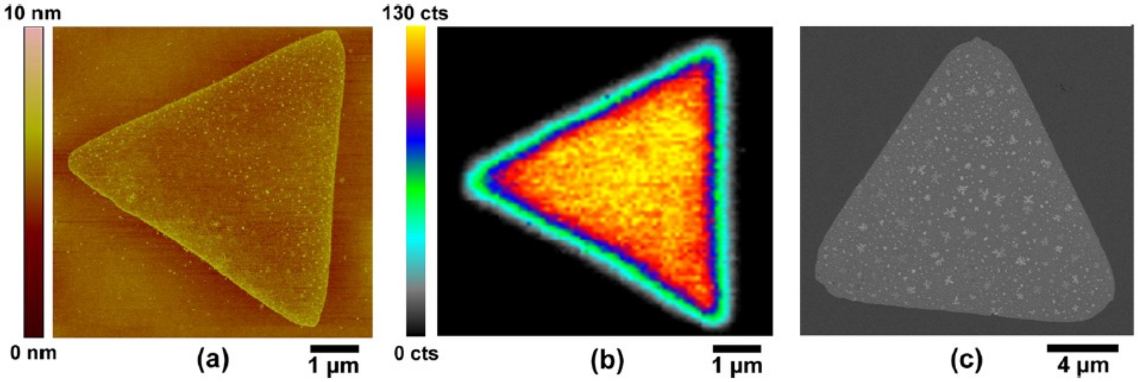

Figure 5. AFM image (a), high resolution Raman map of the out plane mode intensity (b), and a backscatter FE-SEM image (c) of a typical MoS_2 crystal.[5]

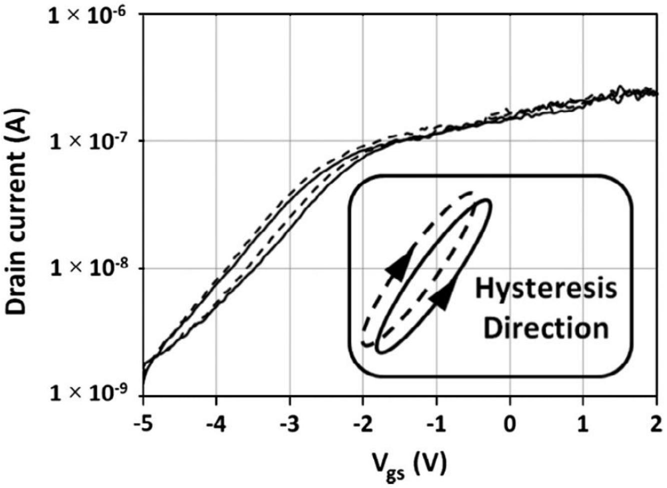

Figure 6. Transfer characteristics at 75 ˥ C. The solid line is for the device before stress, the dashed line for the device after stress. Hysteresis is clockwise for the dashed curves and counterclockwise for the solid line..[5]

3. CONCLUSION

To enable the ever-increasing demand for sensors, communication and computation on the dismounted soldier, we are exploring the properties of novel 2D materials with an eye towards breaking the energy efficiency limit of silicon microelectronics, enable efficient RF technologies and flexible electronics. Our theoretical calculations show that the electronic properties can be engineered with strain, but to date, fabricated devices show performance significantly reduced from the theoretical limits. Our next step is to investigate vertical transport in van der Waals heterostructures consisting of multiple 2D materials in contact with 3D materials to overcome some of the performance limitations of in-plane transport.

It is clear that 2D materials are in the discovery stage in terms of material quality, new 2D materials yet to be explored, and novel device concepts for energy efficient electronics. That said, we believe the path forward for 2D materials is heterogeneous integration with conventional semiconductor technology, such as Si or GaN, where novel devices based on 2D materials will operate in extreme low-power mode, efficient RF devices, or as novel sensors. In addition, 2D materials also show promise for flexible and wearable electronics that could for instance be integrated into soldier uniforms.

4. REFERENCES

[1] Cochran, W. T., del Rosario, R., Wilson, J., Amirtharaj P. and Harjani, R., "Challenges and Opportunities for Energy Efficient Digital Electronics," GOMACtech, (2015).

[2] DARPA: DAHI - Compound Semiconductor Materials on Silicon (COSMOS). Accessed 19 February. http://www.darpa.mil/Our_Work/MTO/Programs/DAHI/Compound_Semiconductor_Materials_on_Silicon_%28COSMOS%29.aspx 2015.

[3] Dong, L., Dongare, A. M., Namburu, R. R., O'Regan, T. P. and Dubey, M., "Theoretical study on strain induced variations in electronic properties of 2H-MoS2 bilayer sheets," Appl. Phys. Lett. 104(5), 053107 (2014).

[4] Lanzillo, N. A., Birdwell, A. G., Amani, M., Crowne, F. J., Shah, P. B., Najmaei, S., Liu, Z., Ajayan, P. M., Lou, J., Dubey, M., Nayak. S. K. and O'Regan, T. P., "Temperature-dependent phonon shifts in monolayer MoS2," Appl. Phys. Lett. 103 (9), 093102 (2013).

[5] Amani, M., Chin, M. L., Birdwell, A. G., O'Regan, T. P., Najmaei, S., Liu, Z., Ajayan, P. M., Lou, J. and Dubey, M., "Electrical performance of monolayer MoS2 field-effect transistors prepared by chemical vapor deposition," Appl. Phys. Lett. 102 (19), 193107 (2013).

[6] Shah, P. B., Amani, M., Chin, M. L., O'Regan, T. P., Crowne, F. J. and Dubey, M., "Analysis of temperature dependent hysteresis in MoS_2 field effect transistors for high frequency applications," Sol.-State Elect. 91, 87-90 (2014).