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The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

15. SUBJECT TERMS

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RPPR Final Report
as of 20-Nov-2018

Agency Code:

Proposal Number: 63801MS **Agreement Number: W911NF-13-1-0364**

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Final Report for Period Beginning 15-Aug-2013 and Ending 14-Aug-2016
Title: 1.2.2. Nanoelectronics and Nanosensors for Army Applications: Hexagonal Atomic Sheets of Silicon (Silicene); Towards Heterogeneous Layered Solids
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Report Term: 0-Other

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STEM Degrees: **STEM Participants:** 1

Major Goals: This research effort focused on pioneering epitaxial synthesis of silicene based on innovative growth approaches and systematic elucidation of the growth kinetics. In addition, fabricated silicene devices was experimentally investigated for the first time in order to shed light on the electronic properties and device physics. The proposed research is organized into three central tasks to address the most pressing challenges facing silicene research.
Task 1: Synthesis of Silicene. The growth of silicene will be accomplished by evaporation of silicon atoms on epitaxial Ag(111) surfaces which offers an hexagonal lattice structure for achieving single-crystal honeycomb films. In addition, alternative transitional metal epitaxial substrates will be investigated that do not react with silicon but can promote epitaxial growth.
Task 2: Experimental Device Studies. Benign wet and dry transfer methods will be investigated including polymer assisted, and direct delamination transfers of the silicene monolayers from the Ag surface to arbitrary insulating substrates for device studies. This task will overcome one of the major barriers to progress regarding material and device studies.

Accomplishments: -Discovery of Ag/mica substrate stack for epitaxial growth of silicene.
-Invention of a method to transfer silicene after growth onto insulating substrates for the first time.
-Demonstration of air-stable encapsulated silicene.
-Demonstration of electrical field-effect control of silicene proving its predicted Dirac properties.

Training Opportunities: Nothing to Report

Results Dissemination: The findings were published in peer-reviewed journals and presented at relevant conferences. The publications and conference are listed in the project attachment report.

Honors and Awards: U.S. Presidential (PECASE) Award from President Obama
Editor, Nature NPJ 2D Materials and Applications
IEEE Nanotechnology Early Career Award

Protocol Activity Status:

Technology Transfer: We established collaboration with ARDEC to study phase transitions in 2D or topological materials. The experimental work was done in synergy with the theoretical/experimental studies performed by Dr. Venkataraman Swaminathan and Mr Dan Kaplan of US-ARMY ARDEC. The samples were prepared by ARDEC scientists who were collaborating with Drs. Patrick Taylor and Patrick Folkes at the Army Research Laboratory. The experimental results obtained at UT-Austin was shared on a regular basis with the ARDEC team to develop a comprehensive understanding of the pressure induced phase transitions in Pb-based IV-VI semiconductors. The ARDEC team visited UT-Austin for extended experiments. A peer-review publication resulted from our joint findings.

Invention Disclosure was filed and patent based on innovative methods to transfer and make silicene devices is pending.

PARTICIPANTS:

Participant Type: PD/PI
Participant: Deji Akinwande
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Li Tao
Person Months Worked: 6.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

ARTICLES:

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Applied Physics
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Volume: 123 Issue: 11 First Page #: 115903
Date Submitted: 11/13/18 12:00AM Date Published: 3/1/18 12:00PM
Publication Location:
Article Title: Structural, vibrational, and electronic topological transitions of Bi
Authors: Joon-Seok Kim, Rinkle Juneja, Nilesh P. Salke, Witold Palosz, Venkataraman Swaminathan, Sudhir Triv
Keywords: 2d materials
Abstract: Topological insulators have been the subject of intense research interest due to their unique surface states that are topologically protected against scattering or defects. However, the relationship between the crystal structure and topological insulator state remains to be clarified. Here, we show the effects of hydrostatic pressure on the structural, vibrational, and topological properties of the topological insulator Bi1.5Sb0.5Te1.8Se1.2 up to 45?GPa using X-ray diffraction and Raman spectroscopy in a diamond anvil cell, together with first-principles theoretical calculations.
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Acknowledged Federal Support: **Y**

RPPR Final Report
as of 20-Nov-2018

PATENTS:

Intellectual Property Type: Patent Date Received: **13-Nov-2018**
Patent Title: Integration of air-sensitive two-dimensional materials on arbitrary substrates for the manufacturing of electronic devices
Patent Abstract: A field-effect transistor and method for fabricating such a field-effect transistor that utilizes an ai
Patent Number: US20180013009A1
Patent Country: USA
Application Date: 13-Jul-2015 Application Status: 2
Date Issued:

ARO Project Summary contents

1. Title of the Proposal, Grant#, PI's Name, Institution

Hexagonal Atomic Sheets of Silicon (Silicene), W911NF-13-1-0364, Deji Akinwande, University of Texas-Austin

2. Objective of the proposal

The objective of this research effort is fundamental growth and investigation of silicene 2D buckled atomic layer than can translate into long-term air-stable silicene materials for basic material physics and device experimental studies. A supplemental research with Army collaborators on phase transitions was also investigated.

3. Technical Approach

Silicene was previously grown on Ag substrates. We determined this was not suitable for down-stream processing for further material studies. We discovered that Ag thin films on mica was a more suitable substrate since the Ag could be removed as a sacrificial layer during transfer and the mica could be recycled for subsequent growth. Afterwards, we developed a completely dry transfer process which protected the silicene layer from chemicals since the silicene is extremely air-sensitive and not robust against common solvents and acids. Lastly we developed an encapsulation layer that protected the silicene in the environment and enabled microfabrication for experimental materials and device studies for the first time.

4. Scientific Accomplishments
-Discovery of Ag/mica substrate stack for epitaxial growth of silicene.
-Invention of a method to transfer silicene after growth onto insulating substrates for the first time (shown below).
-Demonstration of air-stable encapsulated silicene.
-Demonstration of electrical field-effect control of silicene proving its predicted Dirac properties.

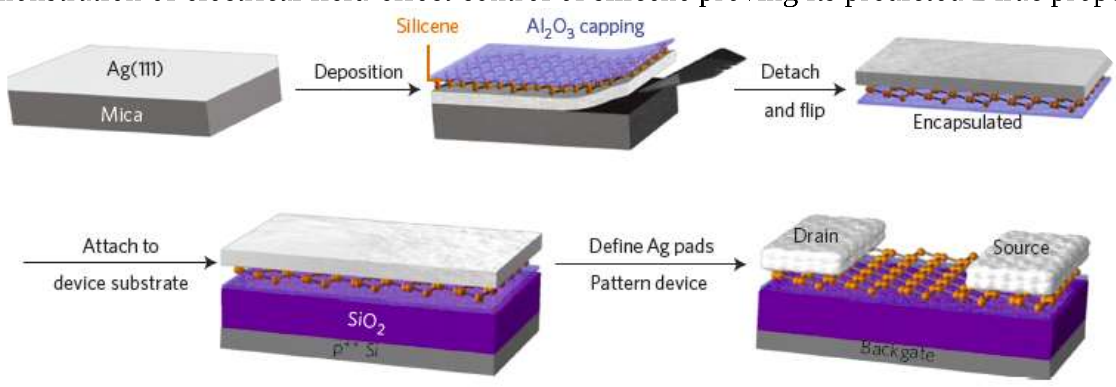

Fig: Invention of a new transfer method named, Silicene Encapsulated Delamination with Native Electrode (SEDNE) that includes the following key steps: epitaxial growth of silicene on crystallized Ag(111) thin film on mica, in-situ Al_2O_3 capping, encapsulated delamination transfer of silicene, and native contact electrodes formation to enable back-gated silicene transistors for the first time.

5. Other Metrics- Tech transfer if any
This project was in collaboration with Army Research Laboratory (ARL) and they engaged in both basic and applied aspects of the properties of this material for Army technology.

6. Any Significant Faculty awards, a list of papers/patents related to this project

Awards

- IEEE Early Career Award in Nanotechnology, 2015
- UT-Austin Jack Kilby Endowed Faculty Fellowship, 2015

Papers

i. J.-S. Kim, R. Juneja, N. P. Salke, W. Palosz, V. Swaminathan, S. Trivedi, A. K. Singh, **D. Akinwande**, and J.-F. Lin, "Structural, vibrational, and electronic topological transitions of Bi1.5Sb0.5Te1.8Se1.2 under pressure," Journal of Applied Physics, vol. 123, p. 115903, 2018.i.

ii. L. Tao, E. Cinquanta, D. Chiappe, C. Grazianetti, M. Fanciulli, M. Dubey, A. Molle, and **D. Akinwande**, "Silicene field-effect transistors operating at room temperature," Nat Nano, Feb. 2015.

iii. **D. Akinwande**, "(Invited) Phosphorene and Silicene: Complexity and Opportunity in Buckled Atomic Sheets," MRS Fall meeting, Boston, Dec. 2015.

iv. **D. Akinwande**, "(Invited) Silicene Field-Effect Transistors," MRS Spring meeting, San Francisco, CA, 2015.

Patent

Li Tao and **Deji Akinwande**, "Integration of Air-Sensitive Two-Dimensional Materials on Arbitrary Substrates for the Manufacturing of Electronic Devices," Invention Disclosure, 2015, Processing by the University of Texas at Austin.

7. Army Relevance: (Army related future applications that you think could be impacted by the current basic research project)
Silicene is a leading candidate for future quantum electronics based on its intriguing topological phase properties, which is a new state of matter discovered in the last decade. The state of matter promises low-energy efficient electronic systems that are protected from scattering by defects and impurities unlike anything seen in other states of matter. Army materials and electronics/sensor technologies stand to benefit with further research and development to exploit this phenomena in silicene and related buckled materials. ARDEC has interest in this type of 2D materials technology and participated in a workshop with the principal investigator and researchers at ARL-SEDD.

7. Army Relevance:
We established collaboration with ARDEC to study phase transitions in 2D or topological materials. The experimental work was done in synergy with the theoretical/experimental studies performed by Dr. Venkataraman Swaminathan and Mr Dan Kaplan of US-ARMY ARDEC. The samples were prepared by ARDEC scientists who were collaborating with Drs. Patrick Taylor and Patrick Folkes at the Army Research Laboratory. The experimental results obtained at UT-Austin was shared on a regular basis with the ARDEC team to develop a comprehensive understanding of the pressure induced phase transitions in Pb-based IV-VI semiconductors. The ARDEC team as well as collaborators from the Army Research Laboratory visited UT-Austin for extended experiments. A peer-review publication resulted from our joint findings. The paper is listed above.