**ABSTRACT**


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**SUBJECT TERMS**

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**SECURITY CLASSIFICATION OF:**
- **a. REPORT** UU
- **b. ABSTRACT** UU
- **c. THIS PAGE** UU
RPPR Final Report
as of 17-Sep-2018

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Report Date: 30-Apr-2017
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Final Report for Period Beginning 01-May-2016 and Ending 31-Jan-2017
Title: SHORT-TERM INNOVATIVE RESEARCH (STIR) PROGRAM:"Synthesizing new functional 2D semiconducting solids"
Begin Performance Period: 01-May-2016
End Performance Period: 31-Jan-2017
Submitted By: Madhusudan Menon
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Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 2
STEM Participants: 0

Major Goals: Experimental synthesis of a new class of 2D material that is one atom thick and flat following the theoretical guidance as part of the exploratory research.

Accomplishments: We attempted the growth of 2D SiC on polycrystalline copper rolls using our Chemical Vapor Deposition (CVD) reactor. During the growth process, both CH4 and SiH4 gases were introduced. The specific objective was to create a stable isolated single layer of the SiC material. The Raman spectrum of the sample grown on copper roll at 1000 C with combined flows of CH4 and SiH4 were analyzed. The TEM images confirmed the presence of both C and Si. Most interestingly, Raman spectrum showed SiC like features in the peaks. These results are significant and confirm growth of at least regions of 2D SiC structures.

Results Dissemination: Nothing to Report

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: Faculty
Participant: Mahendra Sunkara Prof
Person Months Worked: 1.00

Funding Support:

Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:
### Participant

**Type:** Graduate Student (research assistant)  
**Participant:** Rong Zhao  
**Person Months Worked:** 6.00  
**Funding Support:**  
- Project Contribution:  
- International Collaboration:  
- International Travel:  
- National Academy Member: N  
- Other Collaborators:

**Participant**  
**Type:** Graduate Student (research assistant)  
**Participant:** Daniel Jaramillo  
**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:** 5-Submitted  
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**Article Title:** Structural, electronic and mechanical properties of Si2BN under uniaxial strain: an ab-initio study'  
**Authors:** Z. G. Fthenakis and M. Menon  
**Keywords:** nanomechanics, molecular dynamics, first principles calculations  
**Abstract:** Si2BN has been recently predicted theoretically as a new entirely planar 2-dimensional metallic material which is stable even at T> 1000 K. It was also found that it is metallic, with few states at the Fermi level and similar electronic properties at the Fermi level as silicene. In the present work we study its structural, electronic and mechanical properties under tensile strain till the fracture limit and compare them to the corresponding properties for graphene. According to our findings, the metallic character of Si2BN is enhanced as a function of strain, since strain introduces several conduction states into the valence band. Study of its mechanical properties reveals Si2BN to be anisotropic, while exhibiting large values of Young's modulus. Furthermore, structurally it is found to be very robust and comparable to graphene.  
**Distribution Statement:** 1-Approved for public release; distribution is unlimited.  
**Acknowledged Federal Support:** Y
We have attempted growth of 2D SiC on polycrystalline copper foils using our Chemical Vapor Deposition (CVD) reactor as shown in Fig. 1. During the growth process, both CH$_4$ and SiH$_4$ gasses were introduced after annealing the copper substrate in a H$_2$/Ar flow at 1000 °C. However, due to safety reasons and to facilitate slow growth rate, we have used very dilute SiH$_4$ (2 mol. %) in hydrogen. This imposed the restriction of using low concentrations of methane. Our preliminary results showed formation of graphene at ultra-low concentration of methane (<0.5 sccm compared to 20 sccm typically used for graphene synthesis). Since carbon solubility in copper is extremely low compared to that of Si, we maintained SiH$_4$ throughout the cooling process even after the CH$_4$ flow was turned off. Fig. 2 shows (a) low magnification TEM image (b) high magnification TEM image (c) EDX spectrum (d) Raman spectrum of the sample grown on copper foil at 1000 °C with combined flows of CH$_4$ and SiH$_4$. TEM images confirm the presence of layered structure while EDX confirms presence of both C and Si. Most interestingly, Raman spectrum shows SiC like feature (~860 cm$^{-1}$) in addition to typical D, G, and 2D peaks characteristic to graphene. These initial results are encouraging and confirms growth of at least regions of 2D SiC structures. We are planning to perform more in-depth characterization of the material and to reproduce the results.
Under varying conditions for CH$_4$ and SiH$_4$ residency times during the reduction, growth, and cooling processes we synthesized 2D materials which shows an additional Raman peak between the D and G peaks of graphene as shown in Fig. 3. Currently we are trying to understand the origin of this peak with additional characterizations.