様　式　Ｃ－１９、Ｆ－１９－１、Ｚ－１９　（共通）

科学研究費助成事業　　研究成果報告書

令和　３ 年　 ６ 月　 ８ 日現在

機関番号：１７１０２
研究種目：基盤研究(C)（一般）
研究期間：2018～2020
課題番号：１８Ｋ０４９４１

研究課題名（和文）Heavy group III, IV, and V elements triangular lattice atomic layers on semiconductor surfaces - a new kind of 2D Dirac materials

研究課題名（英文）Heavy group III, IV, and V elements triangular lattice atomic layers on semiconductor surfaces - a new kind of 2D Dirac materials

研究代表者
Ａｎｔｏｎ　Ｖ. Ｖｉｓｉｋｏｖｓ（Visikovskiy, Anton）

九州大学・工学研究院・助教

研究者番号：７０４４９４８７

交付決定額（研究期間全体）：（直接経費）　　3,300,000円

研究成果の概要（和文）：周期表の III、IV、および V 族の高密度三角格子 2D 材料は、安定であるとは予想されませんでした。 私たちの研究は、重要な基板相互作用（SiC 基板）により、この形態が最も安定していることを示しています。 これらの物質における電子相互作用は、非常に特異な性質を持っています。 三角形構造にもかかわらず、堅牢なディラック電子分散が形成されます。 スピン偏極状態には 2 種類あります。 今までに見られなかった現象。 これは、電子相互作用における対称性に関する私たちの理解を変えます。 この基本的な特性は、将来のスピントロニクス デバイスで使用できます。

研究成果の学術的意義や社会的意義
新しいクラスの 2D マテリアルが見つかりました。 重要な学術的含意: 電子雲の対称性がさまざまなスピン相互作用をどのようにもたらすかについてのこれまでの理解は完全ではなく、別の考慮事項を考慮に入れる必要があることを示しました。

社会にとって、この結果は重要です。なぜなら、適切な材料生成技術を使えば、この現象を将来の高効率計算デバイスで使用できるからです。

研究成果の概要（英文）：Dense triangular lattice 2D materials of group III, IV, and V of periodic table were not expected to be stable. However, our study has shown that owing to crucial substrate interaction (SiC substrate), this form is most stable compared to conventionally expected honeycomb lattice. The electron interaction in these materials have a very peculiar nature. We still have Dirac-like electronic dispersion, however, unlike in graphene, caused by in-plane orbitals. Spin-orbit interaction results in appearance of two types of spin polarized states. The phenomenon which has been not observed before and change our understanding of symmetry in electronic interactions. Though experiments have been performed on tin layers only, extensive calculations show very large class of materials behaving in similar manner, revealing the fundamental nature of phenomena. With proper material engineering technique, this can open a range of practical applications of these materials in novel spintronic devices.

研究分野：表面物理

キーワード：Spin polarization　Dirac materials　2D layer　semiconductors

１．研究開始当初の背景

(1) Graphene has appeared on the scene of material science and opened the whole new horizons for exotic electronic phenomena. Having Dirac like electron band dispersion happen to play an important role and search for other Dirac materials began. The ones to put a significant hope for were heavier elements with noticeable spin-orbit interaction (SOI), as this may reveal a fascinating physics in spin polarized electrons. Most of the materials that were mimicking graphene's honeycomb structure but consisting of different elements. These were found relatively unstable, hard to grow, and strongly interacting with substrate with their sticking out p_z orbitals – essential ingredient of Dirac dispersion in honeycomb structures, which diminished their exotic properties. So, new type of 2D material with robust Dirac bands and preferably noticeable SOI were in demand.

(2) Group III, IV, and V metals on SiC had long history of forming sparse surface phases, which did show some of interesting physics, such as spin-liquid phase, Mott insulator transition and other phenomena related to strongly correlated electron behavior. However, 2D dense layers of the above materials were not really well studied.

２．研究の目的

The purpose of our research was to resolve some of the issues mentioned above and find interesting systems which could exhibit observable spin polarization as well as robust Dirac electronic structure. The following objectives have been postulated:

* Formation of stable non-honeycomb Dirac material directly on semiconductor surface;
* Triangular lattice atomic layers (TLAL, Fig. 1) are example of so-called frustrated lattices, so such an interesting physics as magnetic frustration, spin liquid state, and spontaneous magnetic ordering can be studied in TLALs;
* As heavy group III, IV and V elements exhibit large SOI, TLALs are expected to have spin-polarized electronic states which are useful for spintronics device application;
* If TLAL is grown at graphene/SiC(0001) interface, one may expect induced spin-polarization of graphene's electronic structure (very useful in spintronics as graphene exhibit long spin lifetimes and diffusion length), and modification of graphene's electronic states caused by moire potential with TLAL;
* The nanostructured TLALs may exhibit some interesting features such as spin-polarized edge states and topological states.

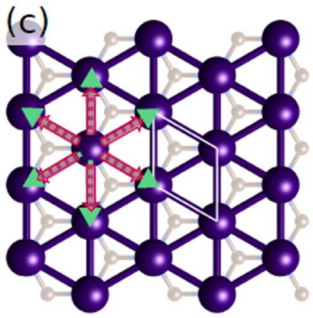

Fig. 1. TLAL

３．研究の方法

To approach the goals of research we applied both experimental as well as computational methods.

The experiments included molecular beam epitaxy (MBE) of the elements onto the surface of SiC(0001), both clean and covered by graphene. The latter technique provided additional advantages, as some elements may intercalate in between SiC substrate and graphene layer and form 2D structures in that confined space, which normally might be unstable on free surface. These structures were then investigates using variety of methods, including low-energy electron diffraction (LEED) for structure determination, atomic force microscopy (AFM) and scanning tunneling microscopy (STM) for morphology and structure analysis, angle resolved photoemission spectroscopy (ARPES) and spin-ARPES for electronic structure. One of the most extensive study, however, has been performed using computational approach using density functional theory (DFT) calculations, because it allows us to predict the stability of various structures and predict the interesting properties which are worth to look for in experiments.

４．研究成果

(1) Experiments have been carried out on graphene/Sn/SiC(0001) system. Originally, the intercalation procedure has been employed to study Sn behavior at the graphene/SiC

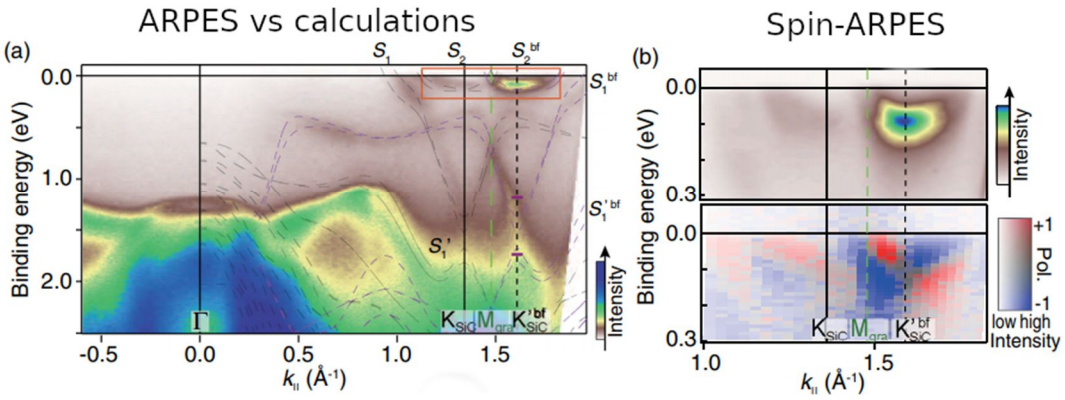

Fig. 2. ARPES and spin polarization

interface, but it was found that (1x1) dense triangular layer is formed. The structure has been determined by LEED analysis and electronic structure has been investigated by ARPES and spin-ARPES (Fig. 2) The results are in excellent agreement with theoretical calculations by DFT, which inspired further investigation of similar systems.

(2) STM results have shown that some higher order periodicity is induced, the origin of which, whether this is just interference with graphene layer or intrinsic structural feature of Sn TLAL is still under investigation.

(3) The extensive computational study on various group III, IV, and V elements have been done. Results show that not all elements have stable TLAL structure on SiC(0001). The stable candidates are Sn, Pb (some buckling of TLAL layer occurs), In, and Sb (Fig. 3).

(4) Calculations show that many elements have gapped Dirac electron bands with various position of Dirac point depending on element. All elements show peculiar double spin polarization of states. Bands originating from p_z orbitals exhibit Rashba-like splitting, while robust Dirac-like states originating from p_x-p_y hybrid orbital show Zeeman-like splitting. This is very unusual behavior. Previously it was believed that type of spin polarization is determined by atomic symmetry of the material. However, our results show that partial electronic charge density symmetry is more important. This is fundamental finding and radically influence our understanding about electronic structure development under SOI.

(5) Possibly the most interesting system is In/SiC(0001). This has spin-polarized Dirac states in the bulk gap of SiC and with Dirac point almost at Fermi level (Fig. 3). This is excellent candidate for spintronic device application. Due to COVID-19 pandemic situation, experiments on this system have been halted for a moment but are planned to resume in future. The calculation results are very promising.

(6) Further study has shown that SiC substrate play significant role in stability of TLAL systems. Introducing another buffer layer, such as silicon nitride cardinally change stability balance and these elements prefer honeycomb structure rather than TLAL, which is the topic of our future research.

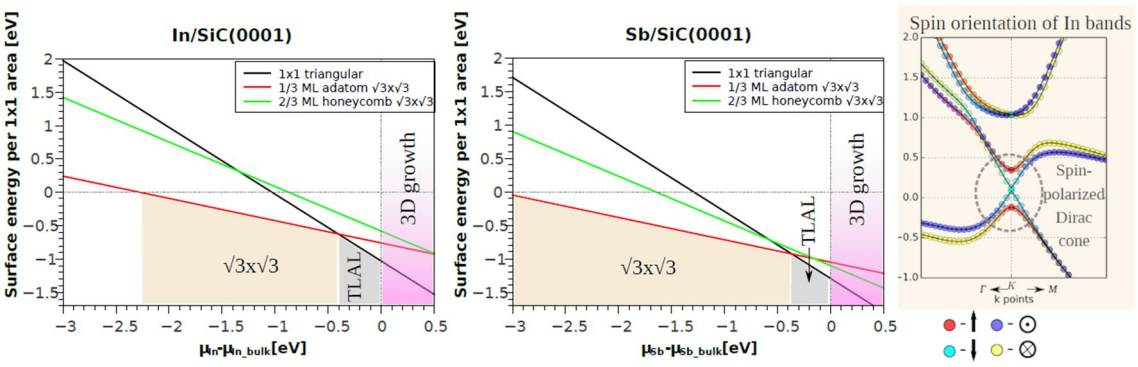

Fig. 3. Stability diagrams of In and Sb, as well as intriguing spin-polarized states in In TLAL system

５．主な発表論文等

〔雑誌論文〕　計3件（うち査読付論文　2件／うち国際共著　3件／うちオープンアクセス　1件）

１．著者名 Yaji Koichiro、Visikovskiy Anton、Iimori Takushi、Kuroda Kenta、Hayashi Singo、Kajiwara Takashi、Tanaka Satoru、Komori Fumio、Shin Shik	４．巻 122
２．論文標題 Coexistence of Two Types of Spin Splitting Originating from Different Symmetries	５．発行年 2019年
３．雑誌名 Physical Review Letters	６．最初と最後の頁 126403
掲載論文のDOI（デジタルオブジェクト識別子） 10.1103/PhysRevLett.122.126403	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 Hayashi Shingo、Visikovskiy Anton、Kajiwara Takashi、Iimori Takushi、Shirasawa Tetsuroh、Nakastuji Kan、Miyamachi Toshio、Nakashima Shuhei、Yaji Koichiro、Mase Kazuhiko、Komori Fumio、Tanaka Satoru	４．巻 11
２．論文標題 Triangular lattice atomic layer of Sn(1 × 1) at graphene/SiC(0001) interface	５．発行年 2018年
３．雑誌名 Applied Physics Express	６．最初と最後の頁 015202～015202
掲載論文のDOI（デジタルオブジェクト識別子） 10.7567/APEX.11.015202	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 Visikovskiy Anton, Hayashi Shingo, Kajiwara Takashi, Komori Fumio, Yaji Koichiro, Tanaka Satoru	４．巻 -
２．論文標題 Computational study of heavy group IV elements (Ge, Sn, Pb) triangular lattice atomic layers on SiC(0001) surface	５．発行年 2018年
３．雑誌名 https://arxiv.org/abs/1809.00829	６．最初と最後の頁 -
掲載論文のDOI（デジタルオブジェクト識別子） なし	査読の有無 無
オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 該当する

〔学会発表〕　計2件（うち招待講演　0件／うち国際学会　1件）

１．発表者名 Visikovskiy Anton, Kajiwara Takashi, Tanaka Satoru
２．発表標題 Stability and electronic structure of novel triangular lattice atomic layers of In, Tl, Pb, and Bi on SiC(0001)
３．学会等名 日本物理学会第73回年次大会（2018年）
４．発表年 2018年

１．発表者名 Visikovskiy Anton, Ando Hiroshi, Hayashi Shingo, Komori Fumio, Yaji Koichiro, Tanaka Satoru
２．発表標題 2D tin layers on SiC(0001)
３．学会等名 第59回 フラーレン・ナノチューブ・グラフェン 総合シンポジウム（国際学会）
４．発表年 2020年

〔図書〕　計0件

〔産業財産権〕

〔その他〕

―

６．研究組織

	氏名 （ローマ字氏名） （研究者番号）	所属研究機関・部局・職 （機関番号）	備考

７．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

８．本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関