Applications of MoS_2 as a Two-Dimensional Material Beyond Graphene

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An article usually includes an abstract, a concise summary of the work covered at length in the main body of the article.

CONTENTS

I. INTRODUCTION

II. GRAPHENE AS A NEW TWO-DIMENSIONAL MATERIAL

A. The Discovery of Graphene

By the end of the last century microelectronics had revolutionized the world, the majority which are silicon-based devices. Today, millions of these silicon-based devices are used in many common electronic devices and have become unavoidable throughout everyday life. Though the first field-effect device was patented in 1925, it was not until 1960 that the first metal-oxide semiconductor field effect transistor was demonstrated [21, 27, 37]. A decade after the first device, devices were being made with several thousand components on a single chip. From there the progress increased at a rapid rate, a process now known as Moore's law, predicting that for each new generation of memory chip and microprocessor unit, the device size would be reduced by 33%, the chip size would be increased by 50%, and the number of components on a chip would quadruple every three years [31, 37]. This proven to be true, and up until recently had shown no signs of stopping. Many times the material limitations were overcome by advances in technology that were seemingly insurmountable and effectively had placed a cap on Moore's law, which ultimately led to new techniques and even more pristine silicon-based materials. However, the limit to oxide thickness has finally placed a maximum on the growth of the silicon-based semiconductor device industy [37]. This impending limit caused many to look for solutions that involved the use of SiO_2 devices and also alternatives to silicon. The result of the latter has given way to a breadth of literature and research that was unforseen a decade before. The search for alternatives to silicon resulted in research into many new, nontraditional materials. Several notable examples are organic conductors and carbon nanotubes [2, 7]. Arguably one of the most interesting nontraditional materials to come out of such research was graphene.

In 1985, with the discovery of fullerenes the amount of known carbon allotropes increased [23, 29]. Fullerenes suggested the existence of a one-dimensional form of carbon, known as carbon nanotubes, which were first demonstrated in 1991 [20]. Despite several theoretical studies involving the use of a single layer of graphite, it was not until 2004 that the first monolayer graphene sheet was isolated [32, 33]. In the most basic sense, graphene is simply a single layer of carbon atoms densely packed into a honeycomb lattice. It is used to describe properties several carbon-based materials (graphite, fullerenes, nanotubes, etc..., see Fig.1) [8, 32, 38]. This was significant because scientists had tried for many years to synthesize monolayers of graphite, though only succeeding in obtaining materials around 10 layers thick [29].

B. Properties of Graphene

To date, graphene's properties have been the focus of much research both theoretical and experimental. Graphene has many unique properties that have paved the way for new subfields in condensed matter physics (i.e. 'relativistic' condensed matter physics). These properties are primarily a result of its low dimensionality and its band structure that allow electrons to mimic relativistic particles [17]. This newly discovered phenomenon has allowed for the study of relativistic effects

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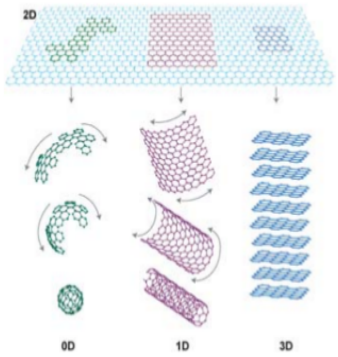

FIG. 1. Graphene can be envisioned in several dimensions. 0-dimensional buckyballs, 1-dimensional nanotubes, or 3-dimensional graphite [35].

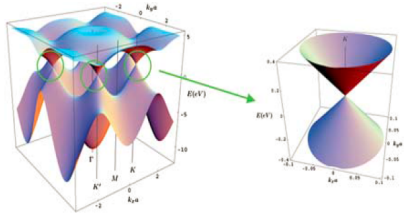

FIG. 2. 3D representation of the electronic band structure of graphene. The right side shows an enlarged view near the Fermi level in one k point [29].

in condensed matter experiements. This includes the appearance of the atypical quantum Hall effect and the confirmation of other relativistic phonomena [34, 45, 51]. However, it is worth noting that this peculiar band structure can be modified by stacking three or more layers of graphene [29].

For applications to electronics a material's band gap is of interest. In graphne, however, the conduction and valence bands touch at a single point as shown in fig. 2 [29, 42]. As a result graphene has no band gap (small band gaps of a few hundred MeV can be introduced in bilayer graphene) [49]. The absence of a band gap is also interesting in the context of the material's optical properties and the implications of these. The absence of a band gap allows for the absorption of light over a large range of the electromagnetic spectrum, ranging from infrared ($< 1.65\,\mathrm{eV}$) to ultraviolet ($> 3.2\,\mathrm{eV}$) giving potential for electronic-photonic device applications [10, 43, 47].

Graphene's mechanical properties have been of much interest over the last decade. Graphene has a Young's modulus of $\sim 1000\,\mathrm{GPa}$ with a breaking stength that is 13% of that [1, 3]. It can also sustain elastic deformations of 20% and due to its two-dimensional nature it has a high pliability [29]. Mechanically, graphene is an exciting material due to the fact that it lies in the extreme ranges of some metrics considering its size and dimensionality.

The mobility in graphene is another property that initially made the material so appealing (and still quite appealing to some degree). Graphene's mobility is about 1000 times that of silicon's [1, 6]. The outstanding crystal quality in larges scale (a few microns) is the major contributing factor here. Without many defects or imperfections the electrons can travel long distances, as much as several micrometers, without being scattered even on rough substrates [9, 29]. The average electron mobility obtained in graphene varies depending on temperature, but the most commonly measured value is $\mu = 100,000\,\mathrm{cm^2V^{-1}s^{-1}}$ with values up to $\mu = 500,000\,\mathrm{cm^2V^{-1}s^{-1}}$ obtainable at low temperatures [15].

III. TRANSITION METAL DICHALCOGENIDES

Graphene is being studied for its unique porperties, however, many other two-dimensional materials are known. Some of the two-dimensional materials being studied in addition to graphene are known as transition metal dichalcogenides (TMDs) [30, 46]. TMDs consist of hexagonal layers of metal atoms (M) in between two layers of chalcogen atoms (X) such that the stoichiometry of the material is MX_2 [49]. The material is dependent on the combination of transition metal, typically one of: Mo, W, Nb, Re, Ni, or V, and chalcogen, typically one of: S, Se, or Te [46]. These materials are commonly are stacked together which involves van der Waals interactions between adjacent sheets and covalent bonding within each individual sheet (see fig. 3) [49]. There are wide variety of properties exhibited by these structures, which include insulator or metal. In addition, they can also display some interesting properties like the topological insulator effect, superconductivity, and thermoelectricity [14, 24, 48, 50]. Ongoing research also includes graphene-like nano materials like silicene and germanene, which are the silicon and germanium-based versions of graphene and are found to show properties that are similar to graphene [4, 41]. These two-dimensional materials are becoming increasingly attractive for a wide-range of applications due to their distinct properties.

A. Properties of MoS_2

As discussed in sec. II B, pristine graphene has no band gap. Though it is possible introduce a band gap in bilayer graphene and graphene nanoribbions, the appeal of many TMDs is that they have direct band gaps which make them ideal candidates for electronic material applications [49]. One such example of a semiconducting TMD is MoS_2 (molybdenum disulphide). TMDs, and

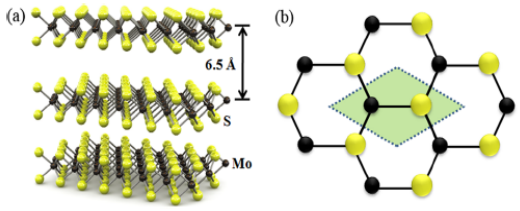

FIG. 3. (a) The atomic structure of layered MoS_2. Different sheets are composed of three atomic layers S-Mo-S, where Mo and S are covalently bonded [36, 49]. (b) Top view of the honeycomb lattice [49].

more specifically MoS_2 and the properties it exhibits have been studided to some extent for several decades with electrical measurements dating back to the 1960s [11, 13]. However, as of late there has been renewed interest in several TMDs are their potential applications.

Like graphene, and many other 2D materials, MoS_2 has a Young's modulus that is comparable to steel ($\sim 205\,\text{GPa}$) [39]. The Young's modulus of single-layer MoS_2 is $\sim 270\,\text{GPa}$. The Young's modulus of bulk MoS_2 is $\sim 240\,\text{GPa}$. The fact that monolayer MoS_2 has a higher Young's modulus than its bulk material counterpart is thought to be mostly due to defects in the material, interlayer sliding, or the absence of stacking faults in monolayer samples [25]. In a further study it was found that the Young's modulus of multilayer MoS_2 ranging in thickness from 5 to 25 layers was $330 \pm 70\,\text{GPa}$ [5]. In addition, both single and bilayer MoS_2 have a breaking strength of about 6% and 11% of their Young's modulus, respectively [3]. This is an indication that MoS_2 is quite flexible compared to other commonly used engineering materials (stainless steel $\sim 0.4\%$, kevlar $\sim 2.6\%$) [16].

As stated before, what MoS_2 and some other TMDs appealing for applications, specifically for use in integrated circuits and logic applications (see sec.V for more on applications). Monolayer MoS_2 has an indirect band gap of $1.8\,\text{eV}$ and few layer (bulk) MoS_2 has a direct band gap of $1.3\,\text{eV}$ [12, 18, 22, 28, 49]. This change in transition from an indirect band gap semiconductor to a direct band gap semiconductor is shown in fig.4. The unusual electronic structure of mono and few-layer MoS_2 which ultimately results in some unique optical properties are due to the composition of the material's conduction and valence bands. The valence band maximum at the Γ point shifts downward to the K point of the Brillouin zone as the number of layers decreases [28, 40]. The change in the band structure as a function of the amount of layers is due to quantum confinement and the change in hybridization between p_z orbitals on S atoms and d orbitals on Mo atoms [26, 28, 40]. Using quantum mechanical modeling systems to investigate the many-body electronic structure of MoS_2 (density functional theory) it has been shown that the conduction

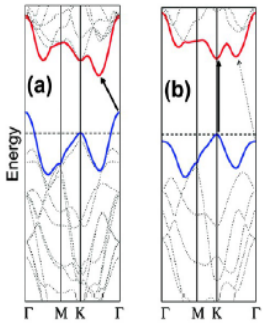

FIG. 4. Calculated band structures of bulk (a) and monolayer (b) MoS_2 and the arrows indicate the lowest energy transition [40].

band states at the K point are primarily the result of d-orbital electrons localized on the Mo atoms in between layers and are relatively unaffected by interlayer coupling [19, 44]. Conversely, states near the Γ-point are strongly affected by interlayer coupling due to the effects of antibonding p_z-orbitals on the S atoms and the d orbitals on the Mo atoms [40]. The result of this is that the states near the K-point are, for the most part, unchanged while the states near the Γ-point are shifted causing the change from an indirect to a direct band gap as the amount of layers of the material is decreased.

IV. SYNTHESIS METHODS

V. APPLICATIONS OF MOS_2

VI. STATE OF THE ART

VII. PROBLEMS AND OUTLOOK

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