Abstract

Tungsten Disulfide (WS_2), a prominent member of the Two-Dimensional (2D) Transition Metal Dichalcogenide (TMD) family, exhibits remarkable properties driven by its unique structural and mechanical characteristics. The atomic structure of WS_2 consists of one Tungsten (W) and two Sulfur (S) atoms arranged in an S-W-S configuration and the atoms are covalently bonded in a hexagonal lattice. Each layer of WS_2 is connected to adjacent layers through weak van der Waals forces. The 2H-phase of WS_2 demonstrates exceptional semiconducting behaviour, characterized by a direct bandgap in its monolayer form and an indirect bandgap in its few-layer configuration. The layer-dependent tunable bandgap, combined with its flexibility and chemical stability, makes WS_2 an outstanding material for diverse applications in both optical and electronic devices. In this research WS_2 is employed as the semiconducting channel, highlighting their potential in electronic applications. As per the application requirements, the material needs to be synthesized with precise control over size, shape, and thickness, as these factors significantly influence its physical and chemical properties. This thesis investigates the synthesis, characterization, and application of 2H-WS_2 nanosheets in back-gated Field-Effect Transistors (FETs).

In the past few decades, various techniques have been reported for the growth of transistor-grade WS_2 nanoflakes. This research focuses on the exfoliation of WS_2 nanosheets through the Liquid Phase Exfoliation (LPE) technique which emerged as a preferred technique due to its simplicity, cost-effectiveness, and eco-friendly nature. This method, often combined with sonication-assisted processes, provides a scalable and efficient approach for producing high-quality WS_2 nanosheets. The study began with the preparation of WS_2 nanosheets via LPE process, using a surfactant acting as an exfoliating agent. This method facilitates the exfoliation of WS_2 nanosheets in an aqueous solution, offering a scalable and environmentally friendly approach. The exfoliated WS_2 nanosheets displayed few-layer structures with thicknesses ranging from approximately 3 nm to 10 nm, as confirmed by spectroscopic and morphological analyses. These measurements also verified the crystalline nature of the WS_2 flakes, which exhibited an

indirect bandgap characteristic of the 2H-phase, making them well-suited for electronics applications.

2H-WS_2 exhibits several extraordinary semiconductive behaviour, nevertheless, it faces challenges in field effect device application due to the presence of an atomic vacancy, low carrier mobility, high contact resistance, etc. Addressing these issues is crucial in the development of high-performing field effect devices. N-type doping with Chlorine (Cl) is employed to improve the stoichiometry of the atomic lattice in WS_2 enabling modulation of its electronic band structure and Contact Resistance (R_C), Schottky Barrier Height (SBH) of Metal-WS_2 contact. The high R_C and SBH can form at the Metal-Semiconductor (M-S) interface which can restrict the carrier transport due to the presence of thick depletion layer. However, n-type doping in WS_2 introduces additional electrons into the semiconductor, increasing the electron concentration in the conduction band. This can aid in reducing the SBH at the Metal-WS_2 interface under bias conditions. In essence, n-type doping modifies the electronic band structure of WS_2 by reducing the depletion region, thereby enhancing carrier transport through tunneling that can make it more conducive. n-type doping of WS_2 with Cl atoms effectively shifts the conduction band closer to the Fermi level, which significantly enhances the material's n-type conductivity. This is attributed to the increase in charge carriers in the conduction band, leading to improved electron mobility and enhanced electrical performance of WS_2. The doping was done through an adsorption process and the effect of doping in the WS_2 nanosheet was confirmed by spectroscopic analysis. The spectroscopic analysis indicates that doping does not modify the surface morphology of the materials. The electrical performance of WS_2 devices was analysed through I-V measurements, revealing that n-type doping significantly improves current conductivity while reducing defects and vacancy states within the nanosheet lattice. Extended doping durations enhanced conductivity, as reflected in the reduction of R_C from 0.35 kΩ to 0.15 kΩ and a decrease in SBH from 0.75 eV to 0.65 eV at the Metal-WS_2 interface. These enhancements enable more efficient carrier transport across the Metal-WS_2 interface, significantly boosting the electrical conductivity of the doped WS_2 nanosheets.

To analyze the properties of Few Layer (FL) WS_2 in FET applications, a back-gated FET was fabricated. The WS_2-FET was constructed on a SiO_2-coated Si substrate, where the SiO_2 layer served as the back-gate dielectric. The fabrication process is done using a contactless lithography technique. The impact of fabrication integrity on the material's properties was meticulously studied using spectroscopic analysis. Electrical characterization of the FET was performed through Current vs. Voltage (I-V) measurements, allowing the extraction of critical parameters such as Field-Effect Mobility (μ_{FE}), carrier concentration, and the on/off current ratio (I_{ON}/I_{OFF}). Furthermore, the influence of metal contact variations, channel length, and doping effects on the electrical properties of FL-WS_2-FETs was comprehensively investigated. The calculated field-effect mobilities for the WS_2-FET were 25.03 $cm^2/V \cdot s$ and 14.3 $cm^2/V \cdot s$, achieved with a pure WS_2 channel of approximately 2 μm in length for Ti and Cr metal contact. After doping, these mobilities increased dramatically to 102.7 $cm^2/V \cdot s$ for Cr contact and ~189.5 $cm^2/V \cdot s$ for Ti contact, attributed to the higher carrier concentration. Additionally, doping led to a reduction in threshold voltage and subthreshold swing across all devices, indicating improved efficiency and switching performance. All the fabricated FETs exhibited n-type behaviour with an impressive I_{ON}/I_{OFF} ratio of ~10^4, demonstrating their suitability for high-performance electronic applications. These findings underscore the potential of FL-WS_2 as a promising material for next-generation FETs, with enhanced performance achievable through careful doping and metal contact engineering.

This research demonstrates the versatility of FL-WS_2 nanosheets as semiconducting materials and highlights the potential in FET application. It further demonstrates that n-type doping of the WS_2 surface significantly enhances the M-S interface, leading to increased carrier concentration and improved device performance. These findings provide a foundation for advancing 2D materials in future semiconductor technologies.

Keywords: *2D; TMD; WS_2; LPE; Doping; SiO_2; Back-gate FET; Metal-Semiconductor interface.*