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Exploring Structural and Optical Traits of WS_2 Films Synthesized through Sulfurization of W and WO_3

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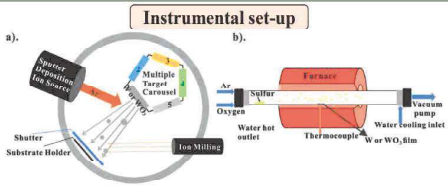
Introduction

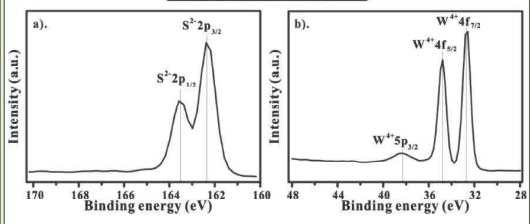
Tungsten disulfide (WS_2) has garnered significant attention due to its unique layer-dependent properties, including its ability to absorb 5–10% of incident sunlight and its distinctive band structure. These characteristics make WS_2 a promising candidate for applications in solar cells, hydrogen evolution reactions, and transistors. However, the efficiency of most WS_2-based devices remains relatively low. In this study, WS_2 was synthesized using ion beam sputtering and sulfurization from tungsten metal (W) and tungsten trioxide (WO_3) across various layer configurations, including monolayer, bilayer, six-layer, and nine-layer structures. To enhance crystallinity, the nine-layer WS_2 was further prepared from tungsten metal and sulfurized in a furnace at different temperatures (800°C, 850°C, 900°C, and 950°C). X-ray diffraction (XRD) analysis revealed that WS_2 exhibited a 2H crystal structure, with crystallinity improving at higher sulfurization temperatures. Moreover, WS_2 prepared from WO_3 (denoted as WS_2-WO_3) demonstrated superior crystallinity compared to that synthesized from tungsten metal (WS_2-W). Raman spectroscopy results showed that the full-width at half maximum (FWHM) of WS_2-WO_3 was narrower than that of WS_2-W, indicating better crystal quality. Furthermore, we demonstrated that high-quality monocrystalline WS_2 thin films could be fabricated at a wafer scale through sulfurization of WO_3. The photoluminescence (PL) of the WS_2 monolayer was strongly enhanced, with a peak centered at 1.98 eV. The WS_2 monolayer also exhibited a transmittance exceeding 80%, and ultraviolet-visible-infrared spectroscopy confirmed its bandgap to be approximately 1.9 eV.

Instrumental set-up



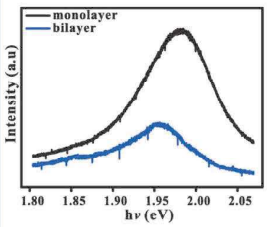
Schematic diagram: a). W-metal and WO_3 prepared on sapphire substrate by ion beam sputtering technique; b). W-metal or WO_3 sulfurization process using a thermocouple-equipped furnace,

Elemental Study



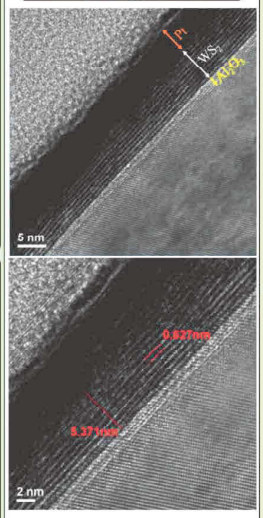
High resolution XPS of WS2 films: (a). S 2P, (b). W 4f and W 5f signals

Micro-PL spectroscopy



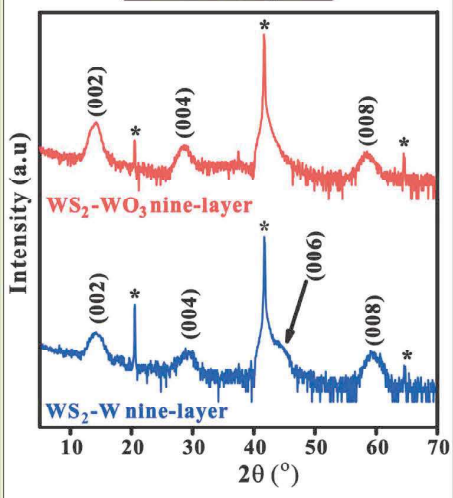
Photoluminescence spectra of WS_2

Morphology Analysis



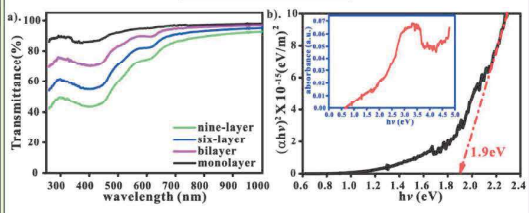
The morphology of the WS_2

Structure Analysis



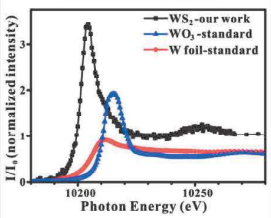
XRD of nine-layer WS_2 sulfurized from W and WO_3 at 900 °C. It shows narrower FWHMs of 002, 004, and 008 signals from WS_2-WO_3

Optical study



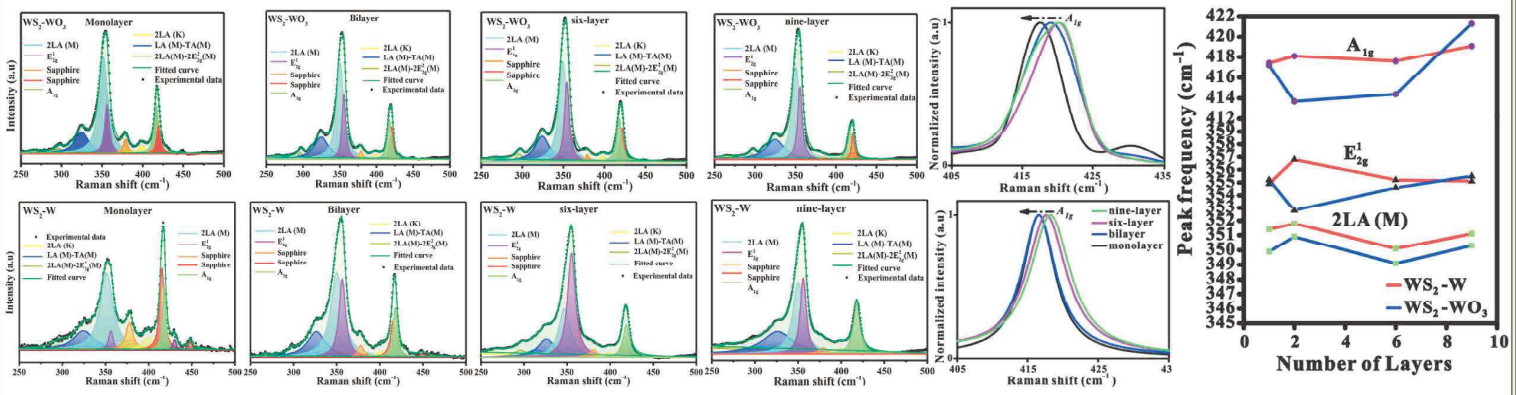
(a) Comparison of the transmittance of the WS_2 thin film with different thicknesses. (b) Band diagram of monolayer WS_2 from the absorption.

XANES Study



The XANES confirmed the structure of WS_2 to be 2-Hexagonal

Raman shift



Raman spectra deconvoluted by Lorentzian fittings of at; WS_2-W (Bottom) and WS_2-WO_3 (Upper). The Raman shift of A_{1g} for WS_2-WO_3 (Upper) and WS_2-W (Bottom). The peaks position of A_{1g}, E^1_{2g}, and **2LA(M)** with respect to the layer number of WS_2.

Conclusions

We report a study of nanoscale WS_2 films prepared by the sulfurization from W and WO_3. The WS_2 films were inferred to be 2H phase and c-axis oriented. The crystal quality of the WS_2 films improved with increasing sulfurization temperature up to 950 °C. X-ray diffraction and Raman spectroscopy show that the FWHM of WS_2-WO_3 is narrower than that of WS_2-W, indicating that the structure of WS_2-WO_3 is superior to that of WS_2-W. The photoluminescence of monolayer WS_2 is strongly enhanced and centered at 1.98 eV. The transmittance of monolayer WS_2 exceeds 80 % and the bandgap is 1.9 eV revealed by ultraviolet-visible-infrared spectroscopy. We conclude that a large-area, high-quality WS_2 film can be prepared by the sulfurization processes of WO_3. The results are promising for applications in next-generation optoelectronic devices.