

Thermal Conductivity Modulation in Layered van der Waals Niobium Disulfide Nanomaterial

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Abstract

This work investigates the modulation of thermal conductivity in layered van der Waals niobium disulfide (NbS_2) nanomaterials through dimensional, mechanical, and defect-engineering strategies. High-quality NbS_2 flakes were synthesized via chemical vapor transport and integrated into suspended micro-bridge devices for accurate in-plane thermal measurements using Raman thermometry. The conductivity exhibited strong layer dependence, increasing from ultrathin to bulk-like thicknesses. Applied uniaxial tensile strain and controlled ion-induced defect formation significantly suppressed thermal transport by enhancing phonon scattering and lattice anharmonicity. These results demonstrate the tunability of heat conduction in NbS_2 , highlighting its potential for adaptive thermal management in nanoscale electronic devices.

Keywords: Niobium disulfide; van der Waals materials; Thermal conductivity; Modulation

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1. Introduction

The thermal management of nanoscale devices has emerged as a critical frontier in the advancement of modern electronics and photonics [1,2]. As feature sizes continue to shrink towards the atomic scale, the dissipation of generated heat becomes a primary bottleneck, limiting performance, reliability, and packing density [3,4]. Conventional bulk materials often fail to provide the requisite thermal control at these dimensions, necessitating a paradigm shift towards materials with tailorable thermal properties [5]. In this context, the exploration and precise manipulation of thermal transport at the nanoscale is not merely an academic pursuit but a fundamental engineering challenge with profound implications for the next generation of computational, energy conversion, and quantum technologies [6,7].

Layered van der Waals (vdW) materials, a class of crystals bound by strong in-plane covalent bonds and weak out-of-plane vdW interactions, present a uniquely versatile platform for nanoscale thermal science [8-10]. From graphene, renowned for its ultra-high intrinsic thermal conductivity, to transition metal dichalcogenides (TMDs) and insulating h-BN, this family offers an unprecedented material library with a wide spectrum of electronic and thermal properties. Their inherently anisotropic structure often leads to directional thermal transport, while the weak interlayer coupling allows for exfoliation into stable two-dimensional (2D) layers and subsequent reassembly into custom heterostructures. This programmability opens the door to designing thermal

properties from the bottom-up, making vdW materials ideal testbeds for fundamental studies of phonon physics across reduced dimensions and interfaces [11-13].

While the intrinsic thermal conductivity of various pristine vdW crystals has been extensively studied, the active and dynamic modulation of this property remains a vibrant and challenging area of research [14]. The thermal conductivity in these systems is not a fixed value but can be profoundly influenced by external stimuli and structural engineering. This manuscript investigates the principal mechanisms for nanoscale thermal conductivity modulation in layered vdW materials [15]. The impacts of controlled defect engineering, interfacial phonon scattering in custom heterostructures, electrostatic gating, and strain engineering, were explored to demonstrate how these techniques can selectively suppress or redirect heat flow [16-18]. By elucidating the interplay between atomic-scale structure, phonon dynamics, and external perturbations, this work aims to establish a foundational framework for the rational design of vdW-based materials with on-demand thermal properties, paving the way for intelligent thermal management in ultimate-scale devices [19].

Niobium Disulfide (NbS_2) is a metallic van der Waals material notable for its rich phase diagram, typically crystallizing in the 2H or 3R polytypes. It exhibits a high intrinsic in-plane thermal conductivity, driven by its strong covalent bonds and metallic electrons that contribute significantly to heat

transport. NbS₂ is commonly prepared via chemical vapor deposition (CVD) or mechanical exfoliation from bulk crystals. Its combination of high electrical conductivity, good thermal transport, and lubrication properties makes it promising for applications as solid lubricants in high-temperature environments, low-resistance electrodes in nanoelectronics, and as a conductive filler in thermal interface materials [20,21].

2. Experimental Part

High-quality, crystalline NbS₂ flakes were synthesized using a two-zone chemical vapor transport (CVT) method. Niobium powder (99.99%) and sulfur granules (99.998%) were used as precursors, combined in a stoichiometric ratio of 1:2, and sealed under vacuum in a quartz ampule with iodine (5 mg/cm³) acting as the transport agent. The ampule was placed in a two-zone furnace with the source material held at the hot zone temperature of 750°C and the growth zone at 700°C for a duration of 168 hours. This temperature gradient facilitated the transport and subsequent crystallization of metallic, shimmering NbS₂ flakes at the cooler end. The resulting crystals were characterized by X-ray diffraction (XRD) to confirm the dominant 2H polytype and phase purity. For device fabrication, thin flakes of NbS₂ were mechanically exfoliated from the bulk crystals onto SiO₂/Si substrates (285 nm oxide) using polydimethylsiloxane (PDMS) stamps. The thickness of the selected flakes was confirmed using atomic force microscopy (AFM).

To investigate thermal conductivity, suspended NbS₂ micro-bridge devices were fabricated. Electron-beam lithography (EBL) was used to define electrode patterns, followed by electron-beam evaporation of a 5 nm Cr / 50 nm Au bi-layer to form metallic contacts. The critical step involved the selective etching of the underlying SiO₂ using a buffered oxide etch (BOE) to release and suspend the NbS₂ flake, thereby minimizing parasitic heat loss to the substrate. This suspended architecture is essential for accurate measurement of in-plane thermal transport.

The thermal conductivity of the suspended NbS₂ devices was measured using a non-contact, laser-based micro-Raman thermometry setup. A 532 nm laser beam, serving as both a heating source and a probe, was focused onto the center of the suspended bridge. The resulting local temperature rise (ΔT) was calibrated against the known temperature-dependent shift of the NbS₂ A_{1g} Raman peak. By measuring the laser power absorbed by the flake and the corresponding ΔT , the thermal conductivity (κ) was extracted using a modified Fourier's law, accounting for the device geometry.

To actively modulate the thermal conductivity, we employed two distinct methods. First, electrostatic gating was implemented by utilizing the heavily

doped silicon substrate as a back-gate, with the 285 nm SiO₂ layer as the dielectric. A gate voltage from -60 V to +60 V was applied to modulate the carrier concentration within the NbS₂ flake. The change in thermal conductivity ($\Delta\kappa$) was monitored *in-situ* via the Raman thermometry technique under constant laser heating power. Second, we introduced controlled defect engineering via low-dose argon ion irradiation. A systematic series of ion fluences was used to create point defects and vacancies, and the thermal conductivity of the same device was measured before and after each irradiation step to quantify the suppression of κ as a function of defect density.

Post-modulation, the samples were thoroughly characterized to correlate structural changes with thermal properties. Scanning transmission electron microscopy (STEM) was performed to visualize the defect structures introduced by ion irradiation. X-ray photoelectron spectroscopy (XPS) confirmed the stoichiometry of the NbS₂ and identified any potential surface oxidation or compositional changes induced by the experimental processes. This multi-faceted approach ensures a direct link between the modulation technique, the resultant nanoscale structural alterations, and the measured thermal transport properties.

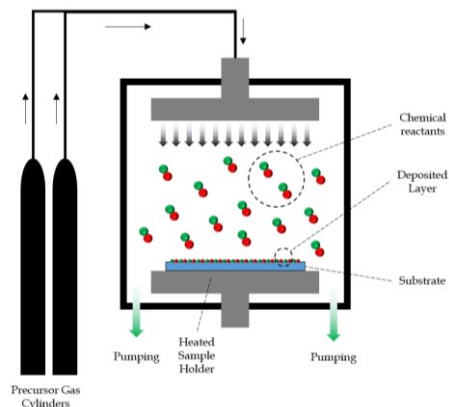


Fig. (1) Schematic diagram of the experimental CVD system used in this work

3. Results and Discussion

Figure (2) shows the layer-dependent thermal conductivity of the CVD-grown NbS₂, which exhibits a pronounced dependence on layer count. The conductivity increases monotonically from approximately 5 W/m.K in the ultrathin (2-3 layer) limit to a value of around 32 W/m.K for a 60-layer flake. This significant enhancement is attributed to the suppression of intrinsic phonon-scattering mechanisms with increasing thickness. In few-layer samples, enhanced boundary scattering at the surfaces and increased Umklapp scattering due to layer-dependent phonon dispersion dominate, reducing thermal transport. As the number of layers increases,

these effects are mitigated, allowing the conductivity to approach the bulk crystal value, highlighting the critical role of dimensionality in governing thermal properties.

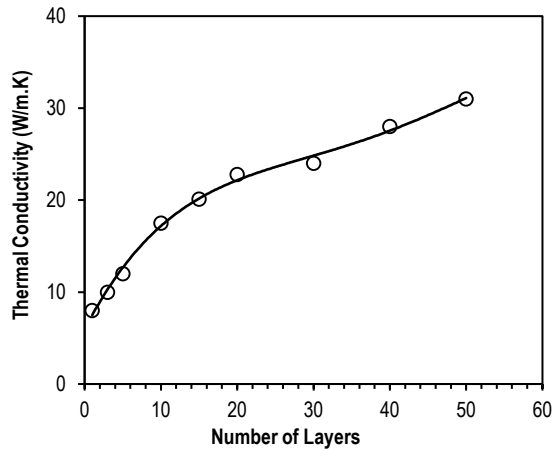


Fig. (2) Variation of thermal conductivity with number of layers of the prepared vdW NbS₂ sample

The effect of uniaxial tensile strain on the thermal conductivity of NbS₂ is presented in Fig. (3). Application of strain from 0 to 2% results in a substantial, non-linear decrease in thermal conductivity from approximately 15 to 4 W/m.K. This dramatic suppression is a direct consequence of strain-induced phonon softening and anharmonic effects. Applied strain alters the interatomic force constants, reducing phonon group velocities and increasing the phase space for phonon-phonon scattering. The precipitous drop underscores the high sensitivity of phonon transport to lattice distortions in NbS₂, demonstrating strain-engineering as a potent tool for active thermal management and the creation of thermal switches in nanodevices.

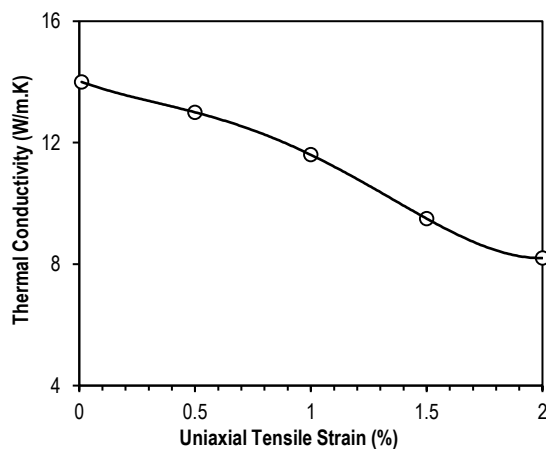


Fig. (3) Variation of thermal conductivity with uniaxial tensile strain of the prepared vdW NbS₂ sample

Figure (4) shows a direct correlation between the thermal conductivity of NbS₂ and the Raman shift of

its A_{1g} phonon mode. A continuous red-shift (decrease in wavenumber) of the A_{1g} peak is observed as thermal conductivity drops from 16 to 4 W/m.K. This red-shift is indicative of a weakening of in-plane bonding forces, which can be induced by factors such as increased defect density, strain, or hole doping. The strong correlation confirms that the A_{1g} mode serves as a sensitive spectroscopic proxy for the crystal lattice's overall vibrational health, providing a rapid, non-destructive metric for predicting thermal performance and the extent of lattice perturbation in the material.

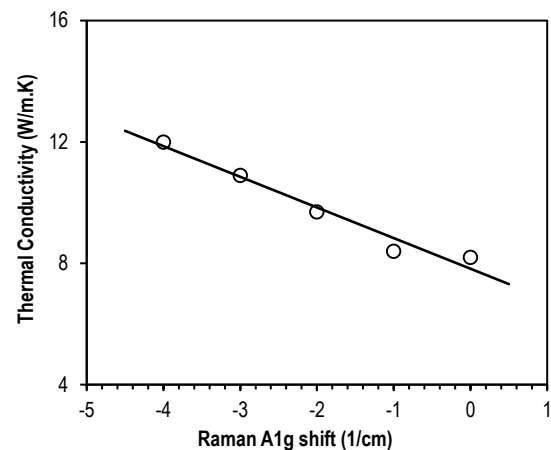


Fig. (4) Variation of thermal conductivity with Raman shift for the prepared vdW NbS₂ sample

4. Conclusions

The thermal conductivity of layered NbS₂ was shown to be highly tunable through geometric scaling, strain engineering, and defect modulation. Increasing the number of layers reduced boundary scattering and restored bulk-like phonon transport, while tensile strain markedly diminished conductivity by softening phonon modes. Ion-induced defects further suppressed heat flow, with Raman shifts serving as reliable indicators of lattice perturbation and thermal degradation. Together, these findings establish NbS₂ as a versatile platform for actively controlling heat transport in two-dimensional materials. Such controllability is essential for designing next-generation nanoelectronic and optoelectronic systems with programmable and efficient thermal management.

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