Nickel particle–enabled width-controlled growth of bilayer molybdenum disulfide nanoribbons

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Transition metal dichalcogenides exhibit a variety of electronic behaviors depending on the number of layers and width. Therefore, developing facile methods for their controllable synthesis is of central importance. We found that nickel nanoparticles promote both heterogeneous nucleation of the first layer of molybdenum disulfide and simultaneously catalyzes homoepitaxial tip growth of a second layer via a vapor-liquid-solid (VLS) mechanism, resulting in bilayer nanoribbons with width controlled by the nanoparticle diameter. Simulations further confirm the VLS growth mechanism toward nanoribbons and its orders of magnitude higher growth speed compared to the conventional noncatalytic growth of flakes. Width-dependent Coulomb blockade oscillation observed in the transfer characteristics of the nanoribbons at temperatures up to 60 K evidences the value of this proposed synthesis strategy for future nanoelectronics.

INTRODUCTION

Reducing the width of two-dimensional (2D) materials toward the quasi-1D nanostructures commonly called nanoribbons (NRs) introduces an additional degree of freedom in engineering their rich electronic behaviors (1–4). The successful synthesis of graphene NRs with controlled edge structures, chirality, and superlattices has generated bandgap opening and tuning, metallicity, topological quantum phases, and Coulomb blockade (CB) (1–5). According to theoretical calculations (6–11), 2D transition metal dichalcogenide (TMD) can also show tunable semiconducting/metallic behaviors, rich band structures, and strong spin-orbit coupling (e.g., MoS2) by adding confinement on width, i.e., making TMD NRs, and controlling the edge structures, which opens another avenue for applications in optoelectronics, spintronics, and quantum computing (12–16). However, unique properties induced by width confinement and edge effects have yet to be validated in 2D TMD NRs because of lack of directly synthesized individual NRs with the appealing width range below \( w \approx 30 \) nm and retained intrinsic properties. Therefore, developing facile methods for width-controlled synthesis of individual 2D NRs of TMDs becomes crucial for further deepening the science and broadening the applications of TMDs.

Currently common fabrication methods rely on top-down techniques such as lithography cutting or etching of monolayer films or flakes (17, 18). Field-effect transistors (FETs) with sub–10-nm monolayer MoS2 channels have been realized through a block copolymer–assisted patterning of MoS2 flakes (19). However, as the electrical performance measured was a collective behavior of multiple sub–10-nm channel lengths, the effect of width confinement was not reflected. More recently, direct growth of monolayer MoS2 ribbons of width down to \( w \approx 50 \) to 100 nm have been realized through a salt-assisted vapor-liquid-solid (VLS) growth (20), as well as a substrate (21) or edge-directed epitaxy process (22). We also previously reported a sodium surfactant–templated growth of MoS2 monolayers with micrometer-scale width (23). However, the properties of these MoS2 ribbons did not show obvious difference from flakes because of still large widths (i.e., \( >50 \) nm). 1D MoS2 channels with \( w \approx 1 \) to 30 nm were grown embedded in other TMD monolayers by taking advantage of dislocations (24) or strain (25) in the lattice, yet exploiting the intrinsic properties of individual, isolated NRs from such channels is difficult. In addition, in analogy to flakes, bilayer NR of 2D materials has another degree of freedom for tunability in interlayer stacking mode and twisting angle, which gives opportunities for discovering new extraordinary properties (26–30). However, bilayer NRs have never been synthesized.

In this work, we present the synthesis of bilayer MoS2 NRs, enabled by Ni nanoparticles, whose diameter controls the ribbon width. The electrical behavior of the NRs shows width dependence, as the achieved true nanorange at \( w \approx 20 \) nm reveals quantum transport behavior, observed even at temperatures up to 60 K, which appears particularly promising for quantum electronic devices.

RESULTS AND DISCUSSION

Growth of bilayer MoS2 NRs

Using an ambient-pressure chemical vapor deposition (APCVD) method in a tube furnace system (fig. S1) (23), ribbon-like MoS2 layers (Fig. 1A) were grown on a SiO2/Si substrate from a mixture of MoO2 + Ni + NaBr powder precursors and S vapor under a moisture-controlled [500 to 3000 parts per million (ppm)] Ar gas flow (for details, see Materials and Methods). The MoS2 ribbons grow to submillimeter lengths (fig. S2A), exhibiting a particular bilayer structure: a wider, up to several micrometers bottom layer and a top layer of much smaller width, \( w < 100 \) nm (Fig. 1A and figs. S3, A and D to F, and S4A). The top-layer ribbon always has, at its tip, a Ni particle (determined by compositional and structural analysis; fig. S7), whose diameter is comparable (usually ~1.1 to 1.6 times larger; see inset of Fig. 1B) to the top-layer width (Fig. 1, A to C). The as-grown MoS2 ribbons were then treated by ultraviolet (UV)
ozone at room temperature in an ambient environment, in which
the exposed bottom monolayer MoS$_2$ was converted to MoO$_3$ (fig. S5)
(31), while the bilayer part of the MoS$_2$ ribbon remained intact
(figs. S3B, S4B, and S6, see the Supplementary Materials for a de-
tailed discussion). The following treatment in a dilute KOH solu-
tion yields bilayer MoS$_2$ NRs (Fig. 1, B to E, and figs. S3C and S4C).
The width of most obtained bilayer ribbons ranges from ~8 to
100 nm, with almost half of the ribbons within 10 to 30 nm
(Fig. 1, B, C, and F), mimicking the distribution of Ni particle diam-
eter (inset of Fig. 1B), apparently defining the ribbon width. Note
that multilayers of MoS$_2$ flakes usually grow underneath the tip Ni
particle (Fig. 1C and figs. S3, G to I, and S7F), which is related to the
growth mechanism of the top-layer NR and will be discussed later.

In the as-grown bilayer MoS$_2$ ribbons, the high-angle annular
dark-field scanning transmission electron microscopy (HAADF-STEM)
reveals a well-identified honeycomb atomic structure in both
mono- and bilayer regions (Fig. 1G). The interlayer stacking, as
seen in the atomic-resolution imaging, is either 2H (Fig. 1G) or 3R
(Fig. 1I) configuration, indicating a homoepitaxy of the top layer on
the bottom layer. The top-layer ribbon appears to grow in an arm-
chair direction but with a mixture of armchair and zigzag edge seg-
ments (Fig. 1, G and I, and fig. S8, A to D), while the wider bottom
layer shows mostly a Mo-terminated zigzag (Mo-ZZ) edge (Fig. 1H
and fig. S8, E and F). The nature edges of the as-grown bilayer ribbons show a certain degree of regularity on both top and bottom
layers [i.e., smooth and straight edges showing uniform armchair
structure (fig. S8A) and Mo-ZZ structure (fig. S8, E and F), respec-
tively]. After UV ozone and KOH treatments, the bilayer MoS$_2$ NRs
retain structural integrity; in particular, neither foreign atom doping
nor damage is observed in the top-layer terrace, although some
damages are observed on the edges (Fig. 1I and fig. S9). NRs of dif-
ferent widths show similar crystallinity (fig. S9).
Growth mechanism of the bilayer ribbon

Seeing clearly that, in the bilayer MoS$_2$ ribbon growth, the crucial role is played by the tip Ni particle, we further explore its composition, evolving during the growth, as Auger electron spectroscopy (AES) reveals: At the very initial stage (i.e., within 30 s after the furnace reaches the growth temperature), the tip particle contains Mo, Ni, Na, S, and O (Fig. 2A and fig. S10), while at the final stage, it is mostly elemental Ni (Fig. 2B and fig. S7). To elucidate the role of different ingredients in MoS$_2$ ribbon growth, we heated the precursor MoO$_2$ + NaBr + Ni mixture (at the same weight ratio and temperature as the ribbon growth) with a SiO$_2$/Si substrate placed above in the growth setup under dry (<100 parts per billion) and moisturized (~500 to 3000 ppm) Ar flow, in the absence of sulfur vapor. Under a dry Ar flow, only NaBr was deposited on the substrate, and there is no indication of reactions within the precursors in the boat according to differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) measurements (Fig. 2D and fig. S11, dashed red curve). However, in the presence of moisture, particles of Na—Mo—Ni—O compounds with an atomic ratio of ~2.0.89:0.13:4.2 estimated by AES spectra (Fig. 2C and fig. S12, A to G) were deposited on the substrate. Corresponding DSC curve (solid red curve in Fig. 2D) exhibits a lower melting point (725°C), indicating the formation of a new compound in the precursors, which could possibly be a Na$_2$MoO$_4$ alloyed with Ni (e.g., Na$_2$Mo$_x$Ni$_{1-x}$O$_4$) as indicated by x-ray diffraction (XRD) patterns (fig. S13). This is also in agreement with the estimated atomic ratio from the AES study (fig. S12G). Sulfurization of the deposited Na—Mo—Ni—O particles (without any additional source) yielded the bilayer MoS$_2$ ribbons (fig. S12, H to J). According to the DSC result, the melting point for the new compound is below the synthesis temperature (770°C), suggesting liquefaction during the growth. Hence, the sufficient level of moisture enables the deposition of the precursors on the substrate. Furthermore, repeating the same set of the growth in the presence/absence of the moisture but without Ni (only MoO$_2$ + NaBr) yielded only typical triangular-shaped MoS$_2$ monolayer flakes (figs. S2, E to J, and S14). Thus, Ni is crucial in promoting the growth of bilayer ribbons, and we next discuss how it leads the process dynamics.

Fig. 2. Growth mechanism study. (A) AES elemental mapping of Mo, Ni, Na, and S, within the terminal area of a bilayer MoS$_2$ ribbon grown for only 30 s. SEI stands for secondary electron image. (B) AES elemental mapping of Mo, Ni, and S, within the terminal area of a bilayer MoS$_2$ NR. The Mo and S detected from the nanoparticle area are originated from MoS$_2$ multilayers precipitated beneath the Ni particle (see also fig. S7). (C) AES elemental mapping of a single particle deposited from a mixture of MoO$_2$ + Ni + NaBr under moisturized Ar flow. (D) DSC curves (highlighting the temperature range from 650° to 800°C) of different precursor mixtures. Solid black, blue, and red curves are NaBr, MoO$_2$ + Ni, and MoO$_2$ + Ni + NaBr under moisturized Ar flow, respectively. The dashed red curve is MoO$_2$ + Ni + NaBr under dry Ar flow. (E) SEM image of an as-grown bilayer MoS$_2$ ribbon. Inset is an enlarged view of the tip area. (F) The width (W) of the bottom layer as a function of its length (L) starting at L = 0 to 150 µm as indicated in (E). The slope (\(\delta W/\delta L\)) of the linear fitting is $-0.046$. 

Li et al., Sci. Adv. 7, eabk1892 (2021) 10 December 2021
To explain the most notable highly anisotropic needle/sword-like morphology of the as-grown bilayer MoS$_2$ ribbon (e.g., Figs. 1A and 2E and fig. S15), one must recognize the dual role of Ni particle in the bidirectional growth (Fig. 3A), resembling the “sonic boom” pattern. The transverse direction of the bottom layer widens with some speed $v$, far from and unaffected by the Ni particle, through a common noncatalytic growth, typical to monolayer MoS$_2$ flakes. After nucleating at the Ni droplet, if nothing else occurred, the bottom layer would grow into a characteristic triangular island. However, the Ni particle moves, while concurrently acting as a catalyst, where the gas feedstock reassembles to yield a top-layer ribbon, which, in turn, propels the Ni particle forward. The signature of generic MoS$_2$ triangles can be discerned in 60° sawtooth edge morphology of the bottom layer (fig. S16), which also suggests that the Ni particle moves not entirely uniformly but in a somewhat on-and-off fashion. Moreover, if the Ni tip is trapped in a trench (intentionally made on the substrate), the longitudinal growth stops, while the bottom layer expands in a triangle (fig. S17), adding an evidence to the two distinct growth mechanisms. The moving Ni droplet nucleates the growth of the bottom layer, which then serves as a perfect template for the homoepitaxial growth of the top layer.

According to the above DSC results, the Ni-contained particle is liquid, so the top ribbon growth is a typical VLS droplet–catalyzed process (32), similar to previously reported nanowires (33), monolayer MoS$_2$ NRs (20), and most common for carbon nanotubes (34, 35). The longitudinal speed ($v$; main growth direction) is driven by this faster VLS mechanism, while the slow noncatalytic transverse widening of the bottom MoS$_2$ layer remains enabled by sufficient supply of feedstock. Indeed, the bottom layer is constantly exposed to feedstock, diffusing toward it across the open substrate surface. In contrast, the concentration of feedstock atop of the bottom MoS$_2$ layer is insufficient to provide for the transverse growth of the top layer. Consequently, the bottom layer exhibits a needle-like shape, while the width of the top layer remains limited to nearly the size of the tip Ni particle. After the reaction stops and during the cooling down, the Ni-contained feedstock droplet solidifies and stops moving, from which the remaining Mo and S precipitate to form MoS$_2$ multilayers underneath the particle (Fig. 1C; fig. S3, G to I; and fig. S7F). Note that as such a precipitation happens during the fast cooling down, the layers do not have time and energy to rotate to the lowest energy orientation, which can result in multilayers with random interlayer twists (fig. S7, F to I). Such a phenomenon is another proof for the VLS growth of the top-layer MoS$_2$ NR (33).

To further quantify the VLS growth mechanism with Ni particles as the catalyst, first-principles calculations were carried out. Constrained molecular dynamics (MD) simulations (36) performed at 1100 K (fig. S18) reveal the catalytic decomposition of MoS$_6$, an immediate molecular gas precursor for MoS$_2$ growth (37), on Ni (111) surface (roughly adequate to represent Ni droplet). The sequential desulfurization results in the formation of ready building MoS$_2$ units for the growth of the MoS$_2$ crystal. Using reaction pathways observed in ab initio molecular dynamics simulations, density functional theory (DFT) calculations (38) were further used to obtain the accurate stepwise decomposition barriers. As shown in Fig. 3B, the overall transformation from the MoS$_6$ to MoS$_2$ unit on Ni (111) is exothermic (~1.86 eV), and the rate-limiting step MoS$_4$ $\rightarrow$ MoS$_3$ has an activation barrier of 0.65 eV, defining the high speed $V$. In addition, fast diffusion of the formed MoS$_2$ unit on the catalyst surface was explained by its computed barrier as low as $\approx$0.25 eV (fig. S19). Furthermore, we calculated the interface energy, which determines how materials nucleate and grow (39) between MoS$_2$ ribbons and the Ni (111) surface. The zigzag edges (both S-ZZ and Mo-ZZ) of MoS$_2$ showed much stronger affinity to the Ni surface (fig. S20), implying that the growth direction must be along the armchair direction, exactly in accordance with our experiments. These results again verify the VLS as the main growth mechanism for the ribbon elongation. Compared to the noncatalytic growth, the VLS growth is much faster because of the catalytic effect of the Ni particles. Our previous study (37) showed a barrier of 0.93 eV for the decomposition of MoS$_6$ and the addition of a MoS$_2$ unit to the kink site of the MoS$_2$ crystal edge (noncatalytic growth, speed $v$). The considerable difference ($\approx$0.28 eV) of the MoS$_6$ decomposition barrier between VLS and noncatalytic growth mechanisms results in the main growth V/$v$ = $e^{0.28eV/kT} \approx 23$ times faster than the secondary transverse growth at the experimental temperature (770°C). This gives rise to [δW/δL] = $v$/$V$ $\approx$ 0.043 slope, in good agreement with the experimentally measured [δW/δL] range of 0.04 to 0.07 (Fig. 2F and fig. S15), further supporting our proposed bidirectional growth mechanism for the bilayer MoS$_2$ ribbons.

Fig. 3. Model and DFT calculations. (A) Schematic illustration of the bidirectional growth of the bilayer MoS$_2$ ribbons. (B) Energy diagram of the catalytic decomposition of MoS$_6$ toward MoS$_2$ unit on the Ni (111) surface. The insets are the relaxed structures of MoS$_6$, MoS$_4$, MoS$_3$, and MoS$_2$ molecules adsorbed on the Ni (111) surface. Yellow, red, and gray balls represent S, Mo, and Ni atoms, respectively. The numbers in parentheses are the nudged elastic band–calculated activation barriers (it is barrierless from MoS$_6$ to MoS$_2$ on the Ni surface), showing a rate-limiting barrier of 0.65 eV.
Electrical performance of bilayer MoS₂ NR

To assess the basic electronics for potential applications, including the role of the width of MoS₂ bilayer NRs, the back-gate FETs (BG-FETs) were fabricated, using Ti/Au as source and drain contacts (see Fig. 4B, inset). Transfer curves of an 8-nm-wide NR device (with 400 nm channel length) were measured at $T = 300$ and 15 K (Fig. 4A). The device shows a typical $n$-type behavior with an ON/OFF ratio of about $10^4$ and a carrier mobility of 4 and 7 cm$^2$/V·s at 300 and 15 K, respectively, calculated using a modified equation considering fringing capacitance induced from ultranarrow NRs (see fig. S21 for a detailed discussion) (40). Arrhenius-like plots of $\ln(I_{ds}/T^{3/2})$ versus $1000/T$ indicate low-energy barrier and, hence, ohmic contact of our NRs (fig. S23) (41, 42), in agreement with the carrier mobilities and linear output characteristics (Fig. 4B and fig. S22) at 300 and 15 K. The good contact allows us to approach the electrical performance reflecting the intrinsic material properties. Notably, the grown bilayer NRs show much higher source-drain current and mobility than those of similar width fabricated by lithography etching from a bilayer flake (fig. S24), demonstrating the advantage of the direct growth method.

To examine the width-dependent transport behavior in the bilayer MoS₂ NRs, we fabricated BG-FETs with a 200-nm-long channel and different ribbon widths (from 8 to 420 nm). At 15 K, prominent periodic oscillations of source-drain current (under 30 mV source-drain bias) as a function of back-gate voltage are only observed for the ribbons no wider than 20 nm (Fig. 4C). The periodic oscillations in the transfer curve, which can be attributed to the CB effect, indicate the quantum dot (QD) behavior of the NR channel (43), made further evident by Coulomb diamonds in the conductance map as a function of $V_{ds}$ and $V_{bg}$ (Fig. 4C, inset, and fig. S25). The width-dependent CB oscillations suggest the essential role of the size confinement by NR width in realizing quantum transport. The presence of a clear diamond pattern indicates that a single QD dominates. By analyzing the Coulomb diamonds (fig. S25), we estimated the energy to add an electron to the QD ($E_{add} \approx 27$ meV), a total capacitance ($C_{tot}$) and gate capacitance ($C_{bg}$) of 5.9 and 0.032 attofarad, respectively, from which the gate coupling factor $\alpha = C_{bg}/C_{tot}$ is $\sim 0.005$. Using the gate capacitance, a QD length of $\sim 1.2$ nm in a 200-nm-long, 20-nm-wide NR can be calculated (fig. S25 and discussion) (44). Temperature dependence measurement of the transfer curves shows that the oscillation remains observable up to 60 K (Fig. 4D). The linear dependence of the FWHM (full width at half maximum) of the oscillation peaks on temperature further confirms the CB behavior (fig. S26), and the slope of the FWHM versus temperature, 0.076,

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**Fig. 4. Electrical performance of bilayer MoS₂ NR-based FET devices.** (A) Transfer curves of an 8-nm-width NR device with 400 nm of channel length under a 100-mV bias at 300 K (red curves) and 15 K (black curves). Solid curves: Linear scale (right y axis). Dashed curves: Logarithmic scale (left y axis). (B) Output characteristics of the device at varying back-gate voltages at 300 K (solid lines) and 15 K (dashed lines). Inset is a typical SEM image of the device. (C) Transfer curves of NRs with different widths (420 to 10 nm) with 200 nm of channel length under a 30-mV bias at 15 K. Inset is the color scale plot of conductance ($G$) versus the back-gate voltage ($V_{bg}$) and source-drain voltage ($V_{ds}$) of the 20-nm-width NR device showing the Coulomb diamonds. The curves are offset for clarity. (D) Transfer curves of the 20-nm-width NR device at temperature from 15 to 60 K. The dashed lines indicate periodic oscillation peaks.
yields the gate coupling factor $\alpha = 0.004$ (fig. S26) (45), close to the value obtained from the Coulomb diamond. So far, CB oscillations in TMDs have been observed only at $T < 4$ K (18, 46–49). Such a strong CB oscillation in our NRs could be due to the very small-sized QD formed in the NR, as the temperature up to which CB oscillations are observable depends on the $E_{\text{add}}$, which increases as QD size decreases. Such effects have been observed previously in carbon nanotubes, leading to similar large charging energies and CB oscillation up to 100 K (44). The observed width-dependent CB oscillation could be attributed to single electron transfer in the MoS$_2$ NRs (43), which is observable up to 60 K. Given the strong spin-orbit coupling in MoS$_2$, the high-temperature quantum phenomena in bilayer MoS$_2$ NRs, enabled by width control by Ni nanoparticles, hold potential for spintronics and quantum computing. Our proposed method for growing bilayer MoS$_2$ NRs could potentially be applied to other TMDs or 2D families by properly selecting combinations of composition of metal particles and growing materials, which will enrich this promising NR platform for quantum electronics.

**MATERIALS AND METHODS**

**Materials synthesis**

The bilayer MoS$_2$ ribbons were synthesized through an APCVD method conducted in a tube furnace system equipped with a 1-inch quartz tube. In the experimental setup, two separate argon gas lines are connected to the tube furnace. One line directly goes to the reaction chamber (called $F_{\text{Ar}}$), while the other goes through a small reaction chamber (called $F_{\text{Ar/H}_2\text{O}}$) before reaching the reaction tube. Therefore, the moisture content in the moisturized Ar carrier gas can be controlled by adjusting the ratio of $F_{\text{Ar}}$($F_{\text{Ar/H}_2\text{O}}$) and measured $F_{\text{Ar/H}_2\text{O}}$ is ~10%, i.e., 72 standard cubic centimeters per minute (scm) of $F_{\text{Ar}}$ combined with 8 scm of $F_{\text{Ar/H}_2\text{O}}$, which accounts for ~3000 ppm of moisture content as measured by a dew point hygrometer (Easidew Online, Rotronic Instrument Corp.) mounted at the inlet to the reaction chamber (fig. S1). For a typical growth run, ~1.5 mg of MoO$_3$ + NaBr + Ni mixture at a certain weight ratio was heated to 770°C, and meanwhile, ~0.1 g of S, placed at the upper stream, was heated to 200°C. The optimum gas flow ratio of $F_{\text{Ar}}$($F_{\text{Ar/H}_2\text{O}}$) is ~10%, i.e., 72 standard cubic centimeters per minute (scm) of $F_{\text{Ar}}$, which combined with ~8 sccm of $F_{\text{Ar/H}_2\text{O}}$, held potential for spintronics and quantum computing. Our proposed method for growing bilayer MoS$_2$ NRs could potentially be applied to other TMDs or 2D families by properly selecting combinations of composition of metal particles and growing materials, which will enrich this promising NR platform for quantum electronics.

**Device fabrication and electrical property measurement**

Electron beam lithography patterning was performed using the Nanobeam n64 Electron Beam Writer system; the electron beam was operated at an accelerating voltage of 80 kV. Metal electrodes of Ti/Au (10/50 nm) were deposited on top of MoS$_2$ NRs in the Angstrom EvoVac Deposition system, and the deposition vacuum level is lower than $5 \times 10^{-7}$ torr. Transport measurements at variable temperature were performed in a CTI Cryogenics model 22 refrigerating a Keysight B1500A semiconductor device parameter analyzer.

**Theoretical calculation**

First-principles calculations based on DFT (38) were carried out using the plane-wave basis Vienna Ab initio Simulation Package (50, 51). The Perdew-Burke-Ernzerhof (52) version of generalized gradient approximation was chosen to describe the electron exchange-correlation interactions, with a cutoff energy of 400 eV. The Ni (111) surface was modeled using a three-layer 6 × 6 supercell slab with the bottom layer fixed. The vacuum layer thickness was ensured to be larger than 10 Å to avoid spurious interactions between neighboring images. Slow growth–constrained MD simulations (36) were performed, with a gradually decreasing distance between Mo in MoS$_2$ and a surface Ni atom, at 1100 K, to mimic the adsorption process of MoS$_2$ on the Ni (111) surface. Canonical ensemble (NVT) using the Nose-Hoover thermostat (53) was used, and the time step was set to 1 fs. The van der Waals interactions were considered for the MD simulation using the DFT-D3 approach (54). Climbing-image nudged elastic band calculations (55) were used, with three to four images between initial and final structures, to obtain the decomposition barriers of MoS$_2$ on the Ni (111) surface. The initial and final structures were fully relaxed using a $2 \times 2$ k-mesh until the force on each unconstrained atom is less than 0.05 eV/Å. To calculate the interface energy between MoS$_2$ ribbons and the Ni (111) surface, a four-layer slab model was used to represent the Ni
(111) surface, with the bottom layer fixed. A ~3.9% compressive strain was applied to Ni to match the MoS2 lattice parameters. The interface energy was calculated as follows: \( E_{\text{interface}} = E_{\text{tot}} - E_{\text{ribbon}} - E_{\text{Ni}} \), where \( E_{\text{tot}} \) denotes the total energy of the MoS2 ribbon/Ni (111) interface, \( E_{\text{ribbon}} \) is the total energy of the MoS2 ribbon, and \( E_{\text{Ni}} \) is the energy of the Ni (111) surface. Spin polarization was considered for all calculations, except MD simulations.

**SUPPLEMENTARY MATERIALS**

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