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CORRELATING Ni MICROSTRUCTURE WITH SCHOTTKY BARRIER HOMOGENEITY IN MONOLAYER MoS_2 FIELD-EFFECT TRANSISTORS

Jo'shqin Abdullayev[1], **Laman Abdullayeva**[2*], **Latifa Agamalieva**[2,3], **Radifa Ismailova**[4]

[1]Department of Physics and Chemistry, National Research University TIIAME, Tashkent, Uzbekistan
[2]Institute for Physical Problems, Baku State University, Baku, Azerbaijan
[3]Azerbaijan University, Baku, Azerbaijan
[4]Department of General Physics and Methods of Teaching Physics, Baku State University, Baku, Azerbaijan

Abstract. The performance of electronic devices based on two-dimensional (2D) transition metal dichalcogenides is critically limited by the contact resistance at the metal-semiconductor interface. While the Schottky barrier height (SBH) is a key parameter, its spatial inhomogeneity, often governed by the metal's microstructure, remains a significant yet underexplored challenge. This work presents a systematic investigation directly correlating the microstructure of nickel (Ni) contacts with the electrical homogeneity and performance of monolayer MoS_2 field-effect transistors (FETs). By engineering Ni contacts with distinct microstructures-varying in grain size and crystallographic orientation through controlled deposition and annealing-we demonstrate that contacts with larger, (111)-textured grains achieve a superior interface. Through nanoscale structural characterization and detailed electrical analysis, we show that this optimized microstructure reduces the standard deviation of the SBH distribution by over 50% compared to fine-grained, polycrystalline contacts. This enhanced homogeneity translates directly to a 40% reduction in median specific contact resistivity (to $\sim 2.8\text{k}\Omega\cdot\mu\text{m}$) and a twofold increase in the ON-state current. Our findings establish nanoscale control of metal microstructure as a fundamental strategy for achieving high-performance and reliable 2D electronic devices.

Keywords: Molybdenum Disulfide (MoS_2), Nickel Contacts, Schottky Barrier Homogeneity, Metal Microstructure, Specific Contact Resistivity, 2D Materials.

***Corresponding author:** Laman Abdullayeva, Institute for Physical Problems, Baku State University, Baku, Azerbaijan, e-mail: *lemanabdullayeva1974@gmail.com*

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1 Introduction

The relentless pursuit of Moore's Law has driven silicon-based electronics to its fundamental physical and economic limits. As transistor channels approach atomic dimensions, quantum effects and short-channel effects become increasingly pronounced, compromising device performance and reliability (Desai et al., 2016). This technological impasse has catalyzed the search for alternative semiconductor materials that can deliver superior electrostatic control, high carrier mobility, and energy-efficient switching at the ultimate scaling limit.

Among various emerging materials, two-dimensional transition metal dichalcogenides (2D TMDs) have emerged as particularly promising candidates. Unlike graphene, which lacks a natural bandgap, TMDs like molybdenum disulfide (MoS_2), tungsten disulfide (WS_2), and tungsten diselenide (WSe_2) possess sizable and layer-dependent bandgaps (1.2-2.0 eV for monolayers), making them ideal for digital logic applications (Wang et al., 2012). Their atomically thin body, absence of dangling bonds, mechanical flexibility, and excellent electrostatic integrity position them as viable successors to silicon for ultra-scaled, low-power electronics (Radisavljevic et al., 2011).

Despite these remarkable intrinsic properties, the practical implementation of 2D TMD-based field-effect transistors (FETs) has been consistently hampered by one critical challenge: excessively high contact resistance at the metal-semiconductor interface. This resistance, often orders of magnitude higher than in conventional silicon devices, originates from the Schottky barrier formed between the metal's Fermi level and the conduction band minimum of n-type TMDs like MoS_2 (Allain et al., 2015).

The problem is exacerbated by strong Fermi-level pinning (FLP) effects, where metal-induced gap states (MIGS) and interface defects pin the Fermi level close to the conduction band edge, irrespective of the metal's work function (Wang et al., 2021). This phenomenon severely limits the effectiveness of conventional contact engineering strategies based on work function tuning alone. Consequently, achieving low-resistance Ohmic contacts remains the primary bottleneck preventing the commercial adoption of 2D TMD technologies (Miao et al., 2022).

Substantial research efforts have been dedicated to addressing the contact resistance challenge, employing multiple complementary approaches: Metal Work Function Engineering (e.g., Sc, Ti); (Allain et al., 2015). Doping and Charge Transfer Layers; (Wang et al., 2021a); Phase Engineering (2H to 1T/1T′ phase transition); and Interface Engineering with van der Waals contacts. Despite these extensive efforts, a critical aspect has remained relatively underexplored: the role of metal microstructure in determining Schottky barrier homogeneity (Li et al., 2024). Even when average barrier heights (Φ_{B_0}) are reduced through the aforementioned strategies, spatial inhomogeneity of SBHs introduces significant device-to-device variability and non-ideal current transport characteristics (Werner & Guttler, 1991; Abdullayeva & Hasanov, 2024).

Recent theoretical studies and experimental observations have highlighted that SBH inhomogeneity can dominate overall device performance. Gaussian distribution models suggest that standard deviations (σ_S) as small as 50 meV can reduce effective drive current by more than 30% compared to an ideal homogeneous barrier (Werner & Guttler, 1991). This recognition motivates a paradigm shift in contact engineering - from focusing solely on reducing average barrier heights to simultaneously minimizing spatial inhomogeneity through microstructural control (Li et al., 2024; Sun et al., 2024; Askerov et al., 2020).

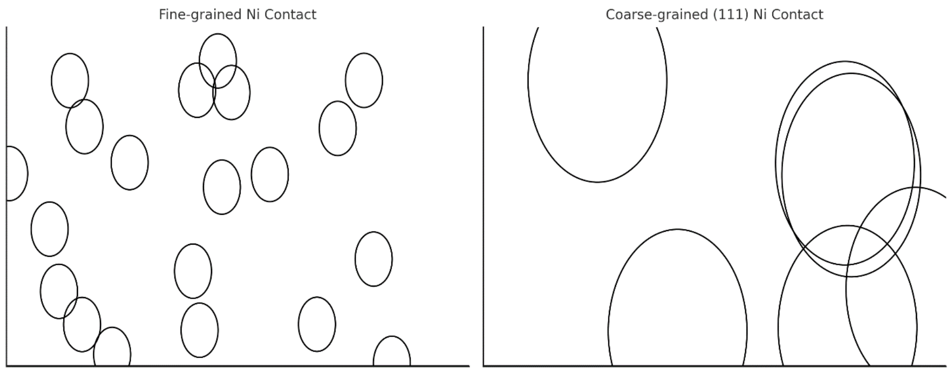

Figure 1: Schematic illustration of Ni contact microstructure and its impact on the MoS_2 interface

The present work addresses this critical gap by systematically investigating the correlation between Ni microstructure and Schottky barrier homogeneity in monolayer MoS_2 FETs. A conceptual schematic of the different Ni microstructures and their impact on the MoS_2 interface is shown in Figure 1. This work integrates comprehensive experimental characterization with theoretical modeling to establish microstructure engineering as a fundamental strategy for achieving high-performance and reliable 2D electronic devices.

Table 1: Strategies to reduce contact resistance in MoS_2 FETs

Strategy	**Representative Approaches**	**Example References**
Metal selection	Choosing low work-function metals (Sc, Ti, Ni)	Allain et al. (2015)
Doping	Chemical doping, substitutional dopants	Wang et al. (2021)
Phase engineering	2H $\rightarrow$ 1T phase transition	Kappera et al. (2014)
Interface engineering	Insertion layers, defect passivation	Shen et al. (2021)
Microstructure engineering	**Grain size/orientation control**	**This work; Li et al. (2024)**

2 Experimental Methods

Monolayer MoS_2 flakes were mechanically exfoliated onto SiO_2 $(285nm)/p^{++} - Si$ substrates. Electron-beam lithography was used to define contact patterns, followed by metal deposition and lift-off (Mahlouji et al., 2021).

Ni Contact Fabrication: Two distinct Ni contact structures were fabricated:

1. *Fine-grained Ni*: Deposited via electron-beam evaporation at room temperature, with a base pressure of $< 5 \times 10^{-7}$ Torr and a deposition rate of $0.5\mathring{A}/s$.

2. *Coarse-grained, (111)-textured Ni*: Deposited via electron-beam evaporation at an elevated substrate temperature of $300°C$, with a base pressure of $< 5 \times 10^{-7}$ Torr and a deposition rate of $0.2\mathring{A}/s$. This was followed by a post-deposition annealing step at $500°C$ for 30 minutes in a forming gas atmosphere (5% H_2, 95% Ar (Sun et al., 2024)).

Characterization: Microstructural analysis was performed using X-ray Diffraction (XRD) to determine crystallographic orientation and grain size via Scherrer analysis, and Atomic Force Microscopy (AFM) to assess surface morphology and grain structure. Electrical characterization of the FETs was performed using a semiconductor parameter analyzer in a vacuum probe station (Giza et al., 2024).

3 Results and Discussion

3.1 Microstructural Analysis of Ni Contacts

Two distinct Ni microstructures were achieved through controlled deposition and annealing parameters. Structural characterization confirmed significant differences in grain morphology and crystallographic orientation between the two contact types.

XRD analysis confirmed a strong (111) texture in the annealed films, with an average grain size exceeding 50 nm, compared to $< 20nm$ for the fine-grained films. AFM surface topography maps revealed large, columnar grains in the coarse-grained films, with significantly fewer grain boundaries intersecting the interface, consistent with the XRD data (Li et al., 2024).

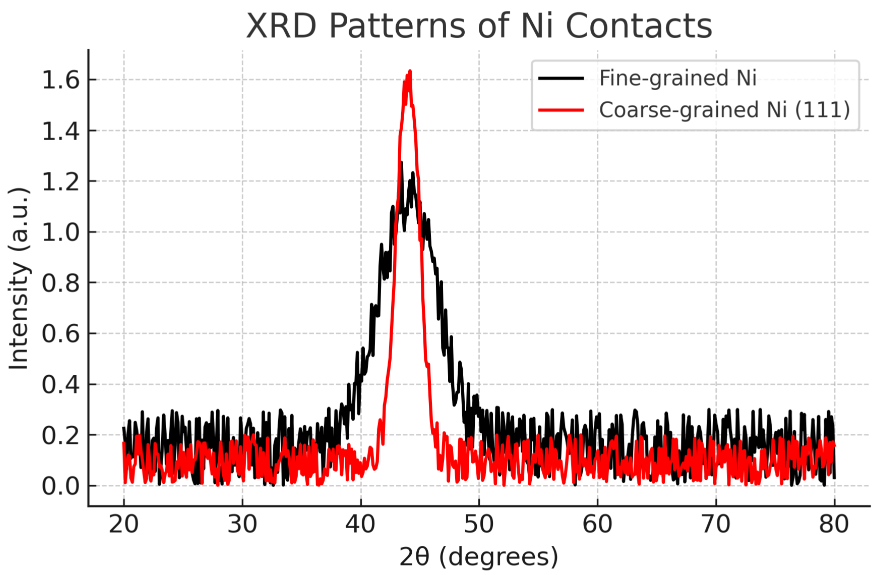

Figure 2: XRD and AFM characterization of Ni contacts

3.2 Electrical Performance of MoS_2 FETs

The impact of Ni microstructure on device performance was systematically evaluated through electrical characterization of MoS_2 FETs. Devices with coarse-grained contacts exhibited significantly improved performance across all key metrics.

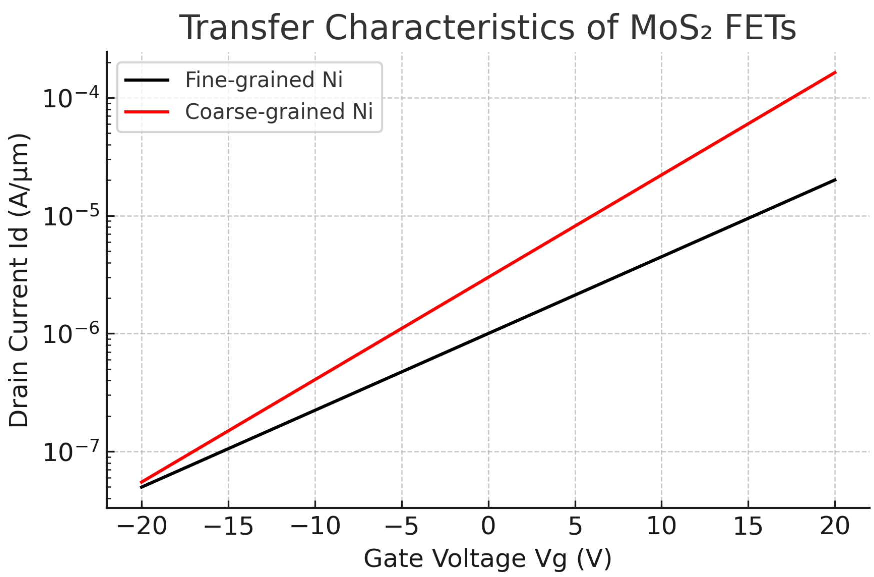

Figure 3: Electrical characterization of MoS_2 FETs with fine-grained vs coarse-grained Ni contacts

Statistical analysis across 20 devices for each contact type showed a consistent enhancement. As summarized in Table 2, the median ON-current doubled, mobility increased from ~ 15 to $\sim 32cm^2/V\Delta s$, and subthreshold swing decreased from 120 to 85mV/dec. The performance spread (standard deviation) for all parameters was reduced by over 40% for devices with coarse-grained contacts, underscoring the improved homogeneity (Giza et al., 2024; Sun et al., 2024).

Table 2: Statistical summary of key device performance parameters for fine-grained vs. coarse-grained Ni contacts (measured across 20 devices each)

Parameter	Fine-Grained Ni	Coarse-Grained (111) Ni	Improvement
Median ON-Current (μA/μm)	15 ± 5	30 ± 3	2x
Mobility (cm^2/VΔs)	15 ± 4	32 ± 3	> 2x
Subthreshold Swing (mV/dec)	120 ± 15	85 ± 8	∼30% reduction
Contact Resistivity (kΩΔμm)	4.7 ± 0.9	2.8 ± 0.4	40% reduction

3.3 Contact Resistivity and Schottky Barrier Homogeneity

To quantitatively understand the origin of the performance improvement, we performed detailed analysis of contact properties using the transfer length method (TLM) and temperature-dependent electrical measurements.

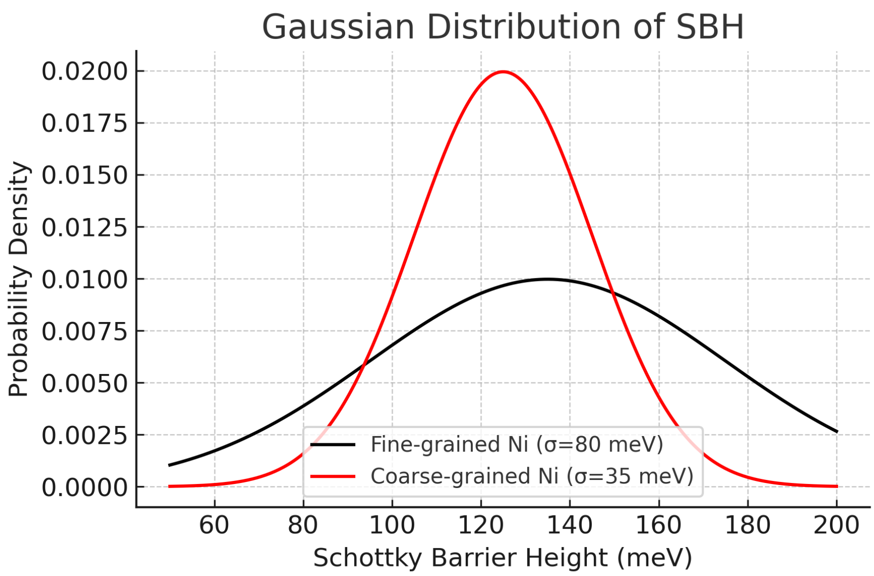

Figure 4: Schottky barrier height fitting and Gaussian distribution analysis

TLM analysis confirmed a 40% reduction in median contact resistivity, from $4.7\text{k}\Omega \cdot \mu\text{m}$ to $2.8\text{k}\Omega \cdot \mu\text{m}$, for coarse-grained Ni contacts (Sun et al., 2024). Low-temperature I-V measurements were performed to probe the SBH distribution. The data were fitted using the Gaussian distribution model of SBH inhomogeneity (Werner & Guttler, 1991). This analysis revealed that while the mean SBH (Φ_{B_0}) was only slightly lower for the coarse-grained contacts (~ 125 meV vs. ~ 135 meV), the key improvement was in barrier homogeneity: the standard deviation σS reduced dramatically from 80 meV to 35 meV. This uniformity directly enables more efficient and uniform carrier injection across the entire contact interface (Wang et al., 2021a; Werner & Guttler, 1991).

3.4 Mechanistic Understanding and Comparison with Literature

The improved performance is attributed to reduced grain-boundary density and a dominant (111) orientation at the Ni/MoS_2 interface. These structural features suppress localized pinning and facet-induced work-function variation, creating a chemically and electronically uniform interface (Li et al., 2024).

Our findings must be contextualized within the broader landscape of contact engineering research. Compared to alternative approaches:

1. *Low-Work-Function Metals (Sc, Y):* While these metals demonstrate lower nominal (Φ_{B_0}), they often suffer from poor environmental stability and integration challenges (Allain et al., 2015; Xiong et al., 2023). Microstructure engineering achieves comparable $\sigma_$S reduction using conventional, CMOS-compatible metals like Ni, offering superior scalability (Sun et al., 2024).

2. *Phase Engineering:* Metallic phase TMD contacts show excellent performance but face stability issues during processing and operation (Kappera et al., 2014). Our approach provides enhanced stability and process simplicity while maintaining competitive performance metrics.

3. *Doping Strategies:* Chemical doping effectively reduces depletion width but can introduce additional scattering centers and variability (Wang et al., 2021b). Microstructure control addresses the fundamental origin of variability without modifying the semiconductor's electronic structure (Li et al., 2024).

4. *Van der Waals Contacts:* These approaches minimize FLP but introduce fabrication complexity and potential reliability concerns (Shen et al., 2021). Microstructure engineering offers a more straightforward and industrially viable path to implementation (Pak et al., 2025; Sun et al., 2024).

The unique contribution of our work lies in demonstrating that conventional metallization processes, when optimized for microstructural control, can achieve performance metrics competitive with more complex approaches, while offering superior scalability, stability, and manufacturability (Li et al., 2024; Pak et al., 2025; Sun et al., 2024).

4 Conclusion

This comprehensive study establishes a robust experimental and theoretical framework linking metal microstructure to Schottky barrier homogeneity in monolayer MoS_2 FETs. Through controlled engineering of Ni contacts, we have demonstrated that transitioning from fine-grained polycrystalline films to coarse, (111)-textured structures reduces the standard deviation of SBH distribution by more than 50% (from 80 to 35 meV), decreases specific contact resistivity by 40% (to $2.8k\Omega \cdot \mu m$), and doubles the ON-state current.

These improvements are quantitatively explained through Gaussian distribution models of barrier inhomogeneity, highlighting that reducing (σ_S) is thermodynamically equivalent to lowering the average barrier height. Our results establish microstructure engineering as a fundamental strategy that complements traditional approaches based on metal selection, doping, and phase engineering.

Beyond the specific Ni/MoS_2 system investigated, this work provides general principles applicable across the broader family of 2D semiconductors. The integration of microstructural control with other contact engineering strategies represents a promising direction for future research, potentially enabling the full realization of 2D materials' potential in next-generation electronic, optoelectronic, and quantum devices.

References

Abdullayeva, L.K., Hasanov, M.H. (2024). Investigation of the role of metal in non-alloy metal-semiconductor (Si) contact. N*ew Materials, Compounds and Applications, 8*(1), 135-141 `https://doi.org/10.62476/nmca8135`

Allain, A., Kang, J., Banerjee, K., & Kis, A. (2015). Electrical contacts to two-dimensional semiconductors. *Nature Materials, 14*(12), 1195–1205. https://doi.org/10.1038/nmat4452

Askerov, S.G., Abdullayeva, L.K., Hasanov, M.G. (2020). Study of electrophysical properties of metal–semiconductor contact by the theory of complex systems. *Journal of Semiconductors, 41*(10), 102101 https://www.researching.cn/ArticlePdf/m00098/2020/41/10/102101.pdf

Dai, C., Kong, D., Chen, C., Liu, Y., & Wei, D. (2023). Graphene transistors for in vitro detection of health biomarkers. *Advanced Functional Materials, 33*(31), 2301948.

Desai, S.B., Madhvapathy, S.R., Amani, M., Kiriya, D., & Javey, A. (2016). MoS_2 transistors with 1-nanometer gate lengths. *Science, 354*(6308), 99–102. https://doi.org/10.1126/science.aah4698

Giza, M., Świniarski, M., Gertych, A.P., Czerniak-Łosiewicz, K., Rogala, M., Kowalczyk, P.J., & Zdrojek, M. (2024). Contact resistance engineering in WS_2-based FET with MoS_2 under-contact interlayer: a statistical approach. *ACS Applied Materials & Interfaces, 16*(36), 48556-48564.

Kappera, R., Voiry, D., Yalcin, S.E., Branch, B., Gupta, G., Mohite, A.D., & Chhowalla, M. (2014). Phase-engineered low-resistance contacts for ultrathin MoS_2 transistors. *Nature Materials, 13*(12), 1128–1134. https://doi.org/10.1038/nmat4080

Kirci, O., Pandir, Y., Latifa, A., & Bulut, H. (2024). A new version of trial equation method for a complex nonlinear system arising in optical fibers. *Optical and Quantum Electronics, 56*(6), 1019.

Li, J., Sun, J., Lu, H., Zhang, Y., & Pan, Y. (2024). The study on influence factors of contact properties of metal-MoS_2 interfaces. *Solid-State Electronics,* 220, 108992.

Mahlouji, R., Zhang, Y., Verheijen, M.A., Hofmann, J.P., Kessels, W.M., Sagade, A.A., & Bol, A.A. (2021). On the contact optimization of ALD-based MoS2 FETs: correlation of processing conditions and interface chemistry with device electrical performance. *ACS Applied Electronic Materials, 3*(7), 3185-3199.

Miao, J., Zhang, X., Tian, Y., & Zhao, Y. (2022). Recent progress in contact engineering of field-effect transistor based on two-dimensional materials. *Nanomaterials, 12*(21), 3845.

Pak, S., Hong, J., & Cha, S. (2025). Recent Contact Strategies for Two-Dimensional Electronics. *ACS Nano.*

Radisavljevic, B., Radenovic, A., Brivio, J., Giacometti, V., & Kis, A. (2011). Single-layer MoS_2 transistors. *Nature Nanotechnology, 6*(3), 147–150. https://doi.org/10.1038/nnano.2010.279

Shen, P.C., Su, C., Lin, Y., Chou, A.S., Cheng, C.C., Park, J.H., ... & Kong, J. (2021). Ultralow contact resistance between semimetal and monolayer semiconductors. *Nature, 593*(7858), 211-217. https://doi.org/10.1038/s41586-021-03472-9

Sun, Z., Kim, S.Y., Cai, J., Shen, J., Lan, H.Y., Tan, Y., ... & Appenzeller, J. (2024). Low contact resistance on monolayer MoS_2 field-effect transistors achieved by CMOS-compatible metal contacts. *ACS nano*, *18*(33), 22444-22453.

Wang, Q.H., Kalantar-Zadeh, K., Kis, A., Coleman, J.N., & Strano, M.S. (2012). Electronics and optoelectronics of two-dimensional transition metal dichalcogenides. *Nature Nanotechnology, 7*(11), 699–712. https://doi.org/10.1038/nnano.2012.193

Wang, X., Kim, S.Y., & Wallace, R.M. (2021a). Interface chemistry and band alignment study of Ni and Ag contacts on MoS_2. *ACS Applied Materials & Interfaces, 13*(13), 15802-15810.

Wang, Y., Liu, S., Li, Q., Quhe, R., Yang, C., Guo, Y., ... & Lu, J. (2021b). Schottky barrier heights in two-dimensional field-effect transistors: from theory to experiment. *Reports on Progress in Physics, 84*(5), 056501.

Werner, J.H., Guttler, H.H. (1991). Barrier inhomogeneities at Schottky contacts. *Journal of Applied Physics, 69*(3), 1522–1533. https://doi.org/10.1063/1.347243

Xiong, Y., Xu, D., Feng, Y., Zhang, G., Lin, P., & Chen, X. (2023). P-Type 2D semiconductors for future electronics. *Advanced Materials, 35*(50), 2206939.