Engineered strain in 2D semiconductor during the growth on grayscale nanopatterned surfaces

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Transistors based on 2D materials, such as MoS_2 , hold promise for logic device scaling due to their sub-nanometer thickness and energy efficiency with low offcurrents. However, they have electron mobilities of 20 to 30 cm²/V·s that fall short of the *International Roadmap for Devices and Systems* projected requirements, $100 \text{ cm}^2/\text{V} \cdot \text{s}$ for 2nm node GAAFETs¹. Strain engineering, successfully applied in commercial Si MOSFETs, is a candidate for enhancing electron mobilities in MoS₂. Promising results including silicon nitride capping² and strain via prestructured substrates³ were introduced. We recently demonstrated up to an 8-fold mobility enhancement in monolayer MoS₂ FETs with 1% tensile strain through the mechanical elongation of the 2D layer during an imprinting process.⁴ All presented approaches where strain is induced on pre-structured surfaces rely on polymer-assisted material transfer from a growth substrate to target surfaces. Such approach faces challenges in nanoelectronics compatibility and scalability, as defects and contamination limit its potential for high-yield production.

As a remedy, we present a new approach in which strain in MoS_2 is introduced *during* its growth process using a grayscale-patterned thin film (patent-pending), instead of a flat substrate. During the cooling phase, the respective surface length change for flat and grayscale (sine-shaped) segments differ due to thermal expansion mismatch between the Si or sapphire substrate and thin film SiO₂. This results in deterministically induced strain in grown 2D materials, depending on the depth-to-pitch ratios of the patterns (Figure 1). Sine-shaped SiO₂ patterns were fabricated using grayscale nanoimprint lithography followed by pattern transfer from resist into SiO₂. The surface roughness was controlled through thermal annealing steps and gentle plasma etching.⁵ Grayscale stamps used for this nanopattern replication were made by thermal scanning probe lithography and dry etching. The CVD-grown MoS₂ on the sine-shape surface resulted in up to 0.8% tensile strain, which is known to improve FET mobilities⁴ to >100 cm²/V·s, confirmed by the 40 meV photoluminescence (PL) peak shift (Figure 2). The presented approach that combines grayscale lithography and transfer-free strained growth of 2D materials is CMOS-compatible, scalable, and allows for reproducible fabrication of strain-engineered high-mobility FET channels.

^{1.} IEEE International Roadmap for Devices and Systems (IRDS), *IRDSTM 2023: More Moore*, p. 12. Available: https://irds.ieee.org/

^{2.} Jaikissoon, M. *et al.* CMOS-compatible strain engineering for monolayer semiconductor transistors. *Nat. Electron.* **7**, 885–891 (2024).

^{3.} Liu, T. et al. Crested two-dimensional transistors. Nat. Nanotechnol. 14, 223–226 (2019).

^{4.} Liu, X. *et al.* Deterministic grayscale nanotopography to engineer mobilities in strained MoS₂ FETs. *Nat. Commun.* **15**, 6934 (2024).

^{5.} Erbas, B. *et al.* Combining thermal scanning probe lithography and dry etching for grayscale nanopattern amplification. *Microsyst. Nanoeng.* **10**, 1–10 (2024).



of grayscale pattern p: picto of sine wave d: depth of sine wave f: surface length of sine w

details.



Figure 2: Photoluminescence (PL) mapping of MoS_2 grown on flat and grayscale nanopatterns fabricated on (a) thermal SiO_2 on silicon (surface fully covered) and (b) PECVD SiO_2 on sapphire (isolated triangular or merged flake). (c) AFM image, showing conformally grown MoS_2 on the pre-patterned substrate from (a). (d) Calculated strain values vs depth-to-pitch ratio (dashed line) and measured PL energy peak shifts vs depthto-pitch ratio.