

SUPPLEMENTAL FIGURES AND FIGURE CAPTIONS

Title: Origins of Ripples in CVD-Grown Few-layered MoS₂ Structures under Applied Strain at Atomic Scales

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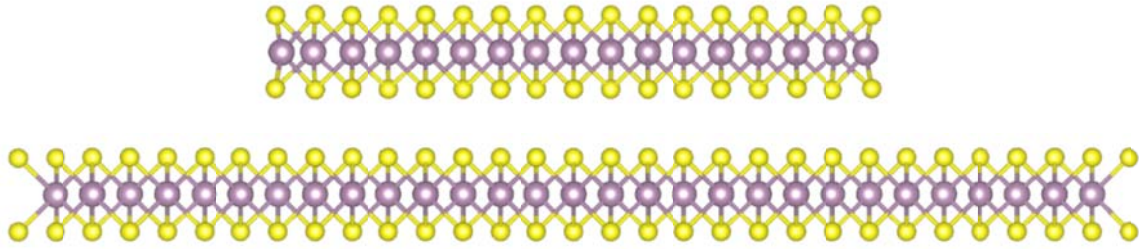


Figure S1: Schematic show of the bilayer supercell used in this study.

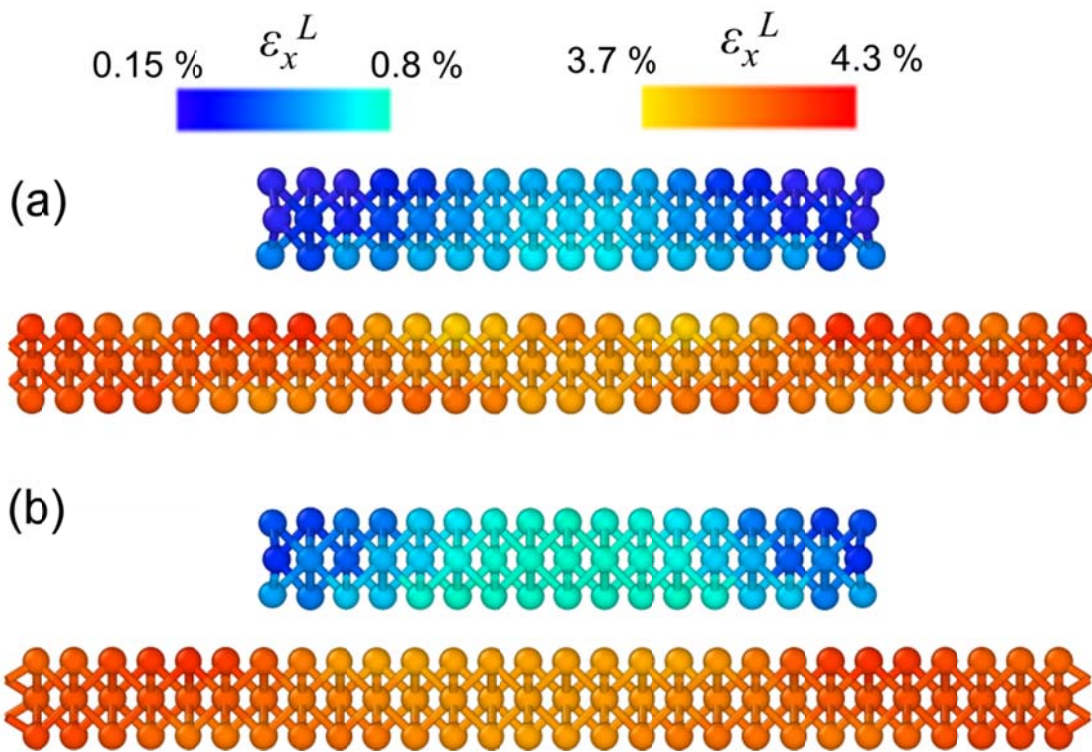


Figure S2: Comparison of (a) DFT and (b) MD in local strain (ϵ_x^L) map of a bilayer MoS₂ system under an applied uniaxial strain $\epsilon_x=4\%$.

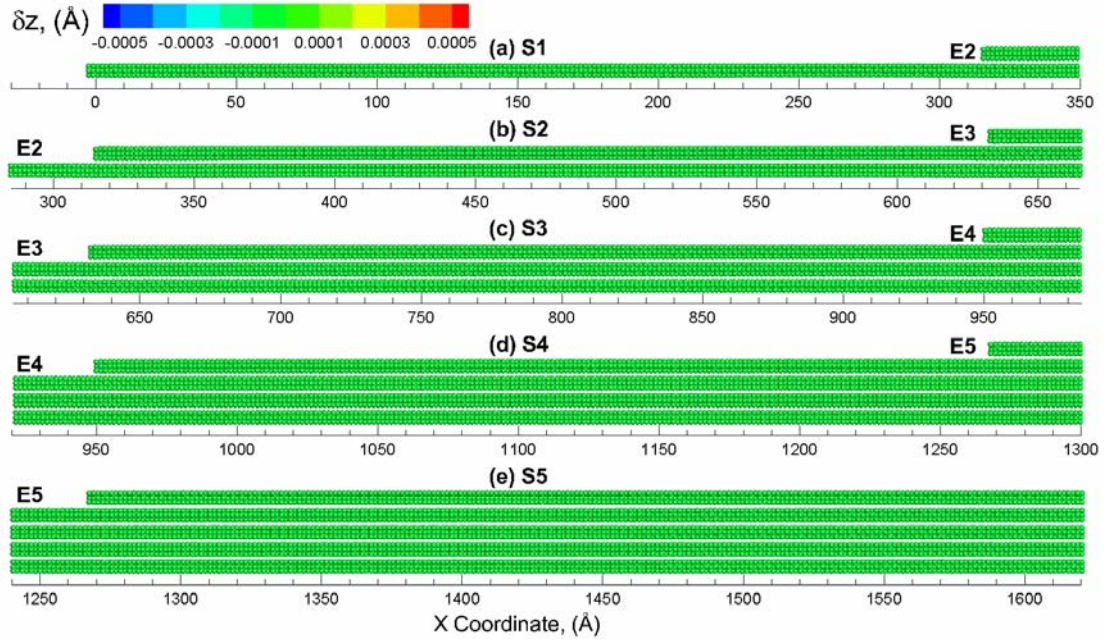


Figure S3: The vertical displacement map in the unstrained configuration at different sections: (a) S1, (b) S2, (c) S3, (d) S4 and (e) S5. The atoms are colored by the displacement in the Z direction with the positive value (red color) corresponding to an upward displacement and a negative value (blue) indicating a downward displacement as compared to the unstrained configuration.

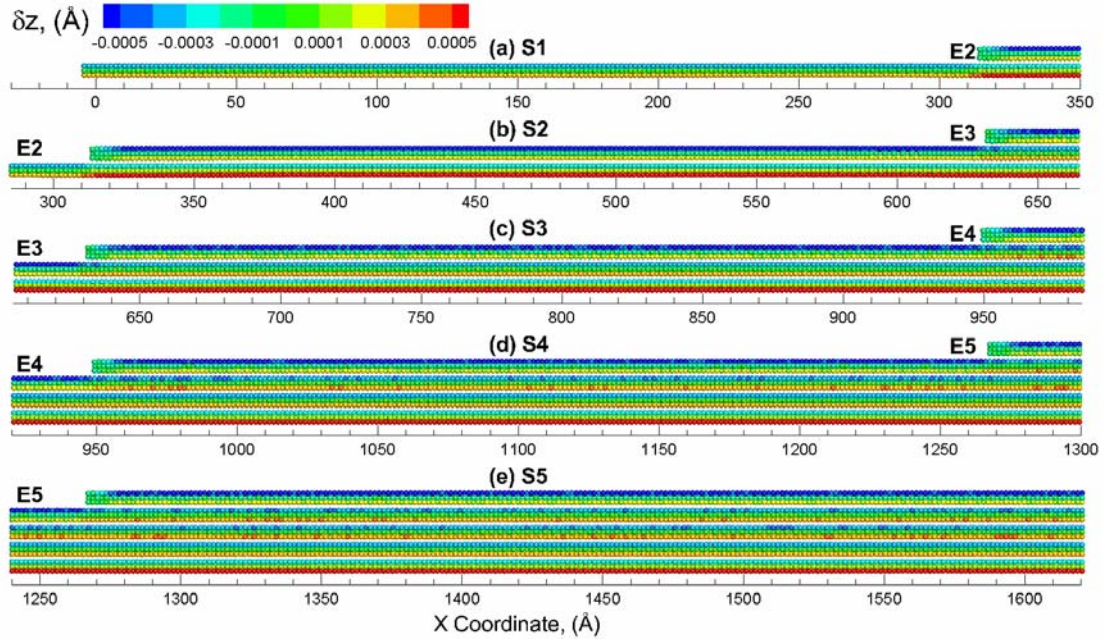


Figure S4: The variation of the vertical displacement in the various sections (a) S1, (b) S2, (c) S3, (d) S4 and (e) S5 of the multilayered structure at an applied strain of $\varepsilon_x = 0.1$ %. The atoms are colored by the displacement in the Z direction with the positive value (red color) corresponding to an upward displacement and a negative value (blue) indicating a downward displacement as compared to the unstrained configuration.

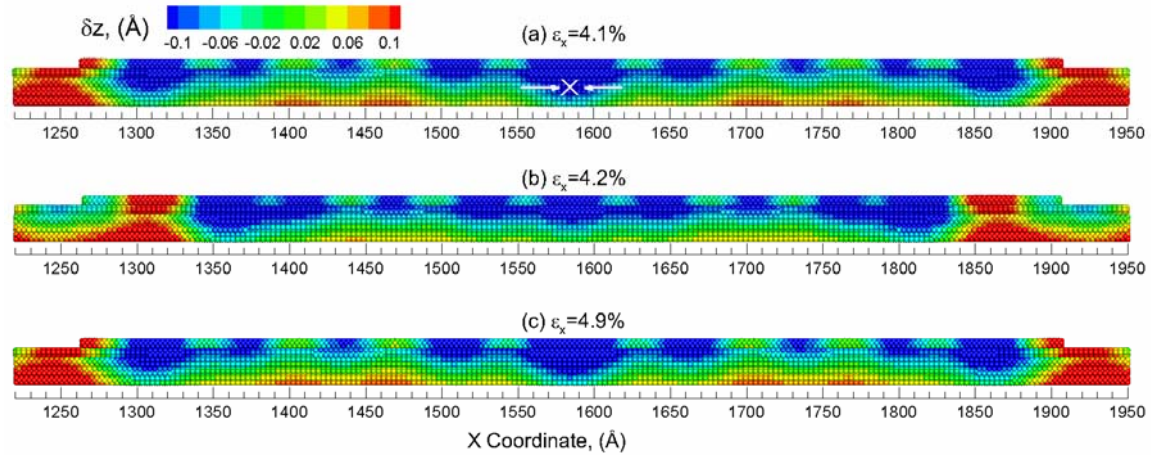
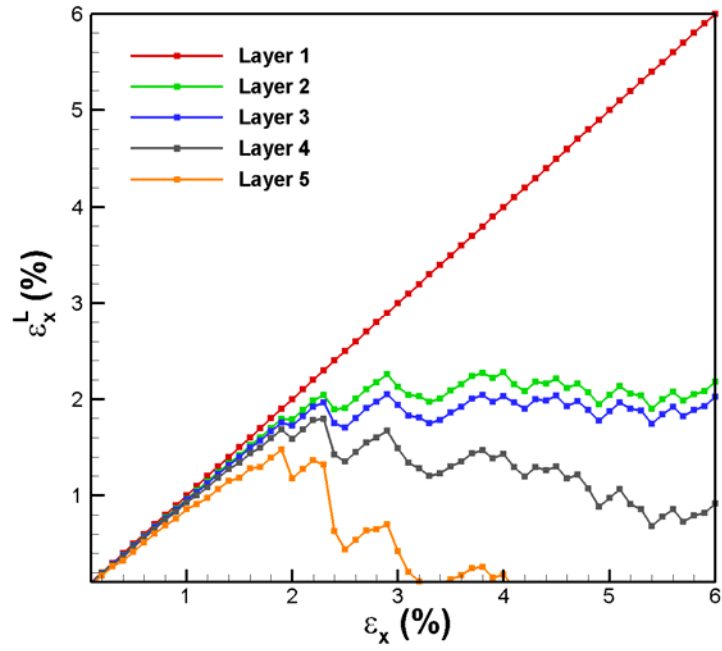
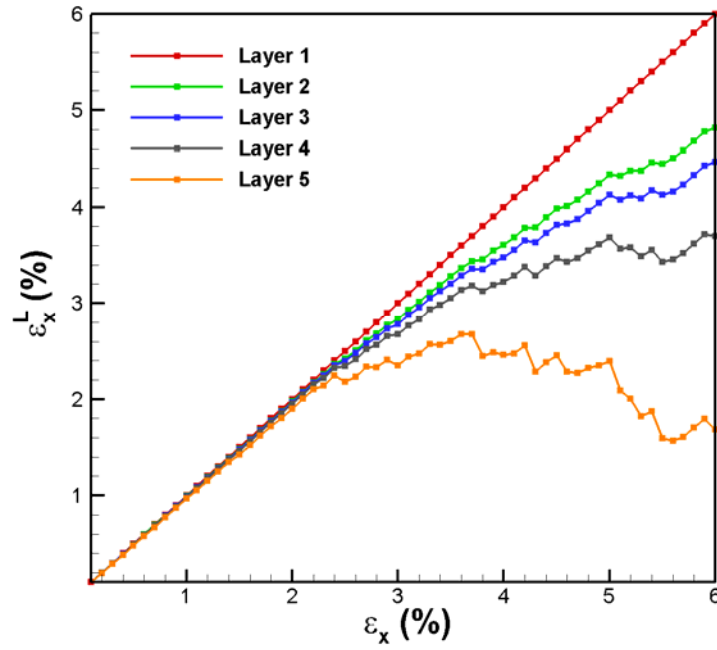


Figure S5: Snapshots of center of pyramid system at various strains (a) $\epsilon_x = 4.1\%$, (b) $\epsilon_x = 4.2\%$ and (c) $\epsilon_x = 4.9\%$ showing propagation of ripples at the edge region. The atoms are colored by the displacement in the Z direction with the positive value (red color) corresponding to an upward displacement and a negative value (blue) indicating a downward displacement as compared to the unstrained configuration.



(a)



(b)

Figure S6: Local layer strain ε_x^L as a function of applied strain ε_x for (a) 127 nm, (b) 634 nm as-grown multilayered MoS₂ structure under uniaxial tensile strain.