

Supplementary Material to
Mechanical properties of MoS₂ nanotubes under tension: a molecular dynamics study

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I. Stress-strain and strain energy graphs of nanotubes of 60 and 80 Å of diameter

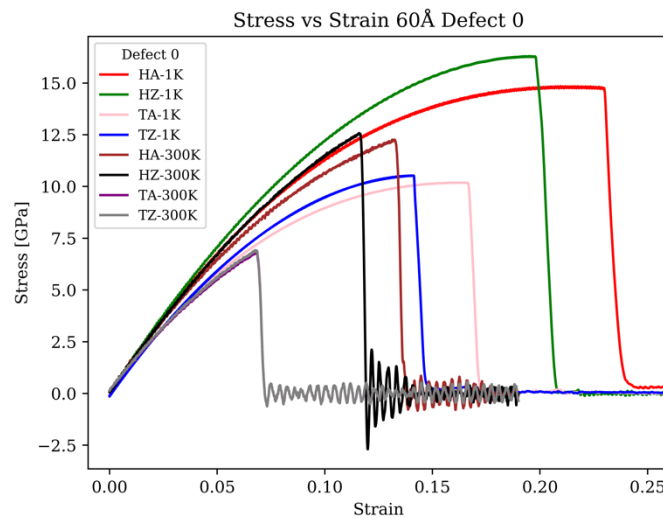


Fig. SM1. Stress-strain curves for defect-free MoS₂ nanotubes of 60 Å of diameter, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

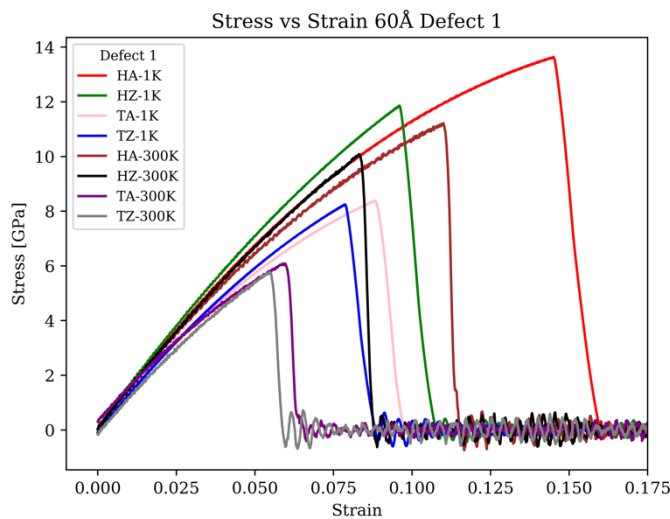


Fig. SM2. Stress-strain curves for MoS₂ nanotubes of 60 Å of diameter, with a defect of kind 1, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

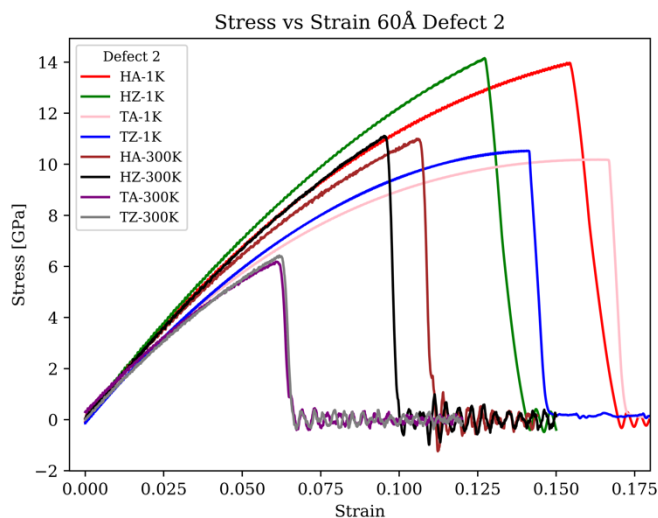


Fig. SM3. Stress-strain curves for MoS2 nanotubes of 60 Å of diameter, with a defect of kind 2, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

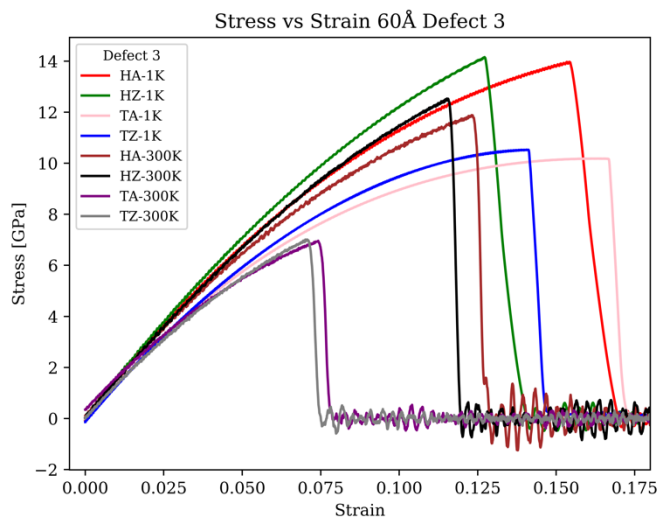


Fig. SM4. Stress-strain curves for MoS2 nanotubes of 60 Å of diameter, with a defect of kind 3, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

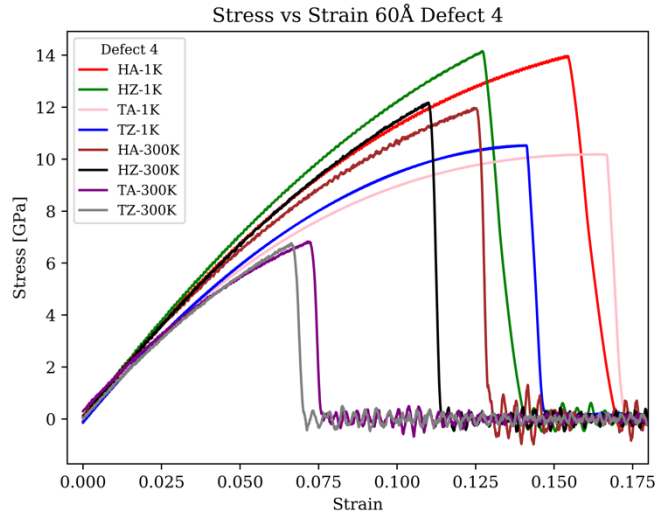


Fig. SM5. Stress-strain curves for MoS₂ nanotubes of 60 Å of diameter, with a defect of kind 4, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

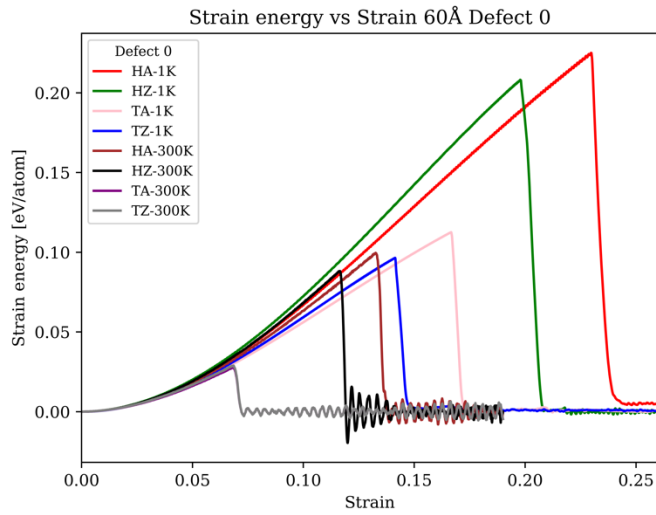


Fig. SM6. Strain energy vs strain curves for defect-free MoS₂ nanotubes of 60 Å of diameter, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

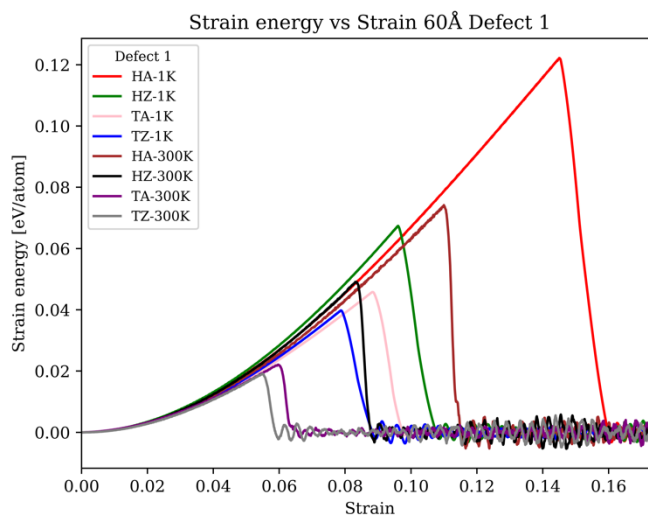


Fig. SM7. Strain energy vs strain curves for MoS₂ nanotubes of 60 Å of diameter, with a defect of kind 1, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

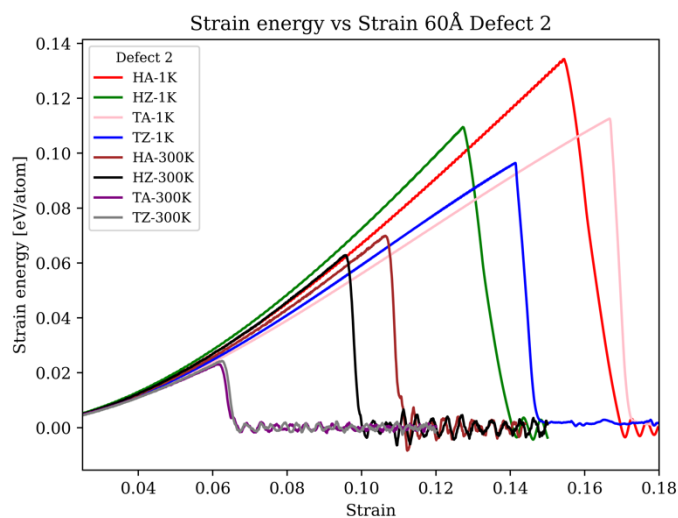


Fig. SM8. Strain energy vs strain curves for MoS₂ nanotubes of 60 Å of diameter, with a defect of kind 2, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

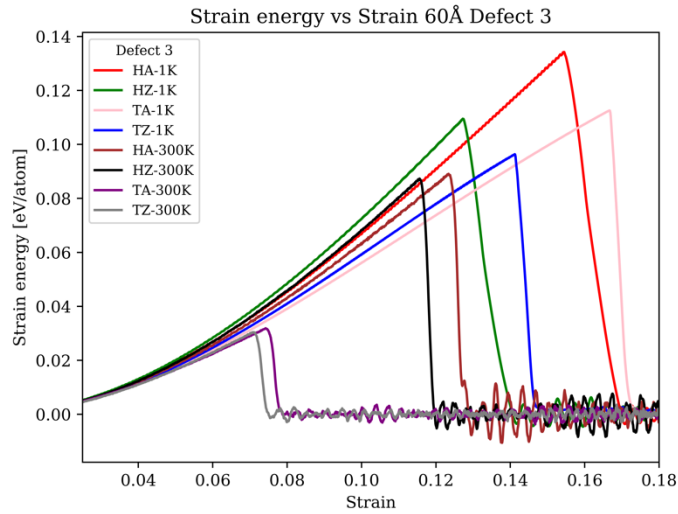


Fig. SM9. Strain energy vs strain curves for MoS₂ nanotubes of 60 Å of diameter, with a defect of kind 3, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

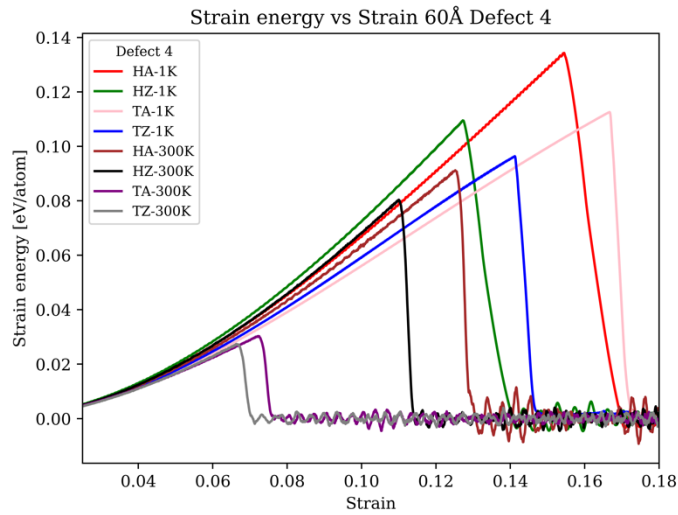


Fig. SM10. Strain energy vs strain curves for MoS₂ nanotubes of 60 Å of diameter, with a defect of kind 4, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

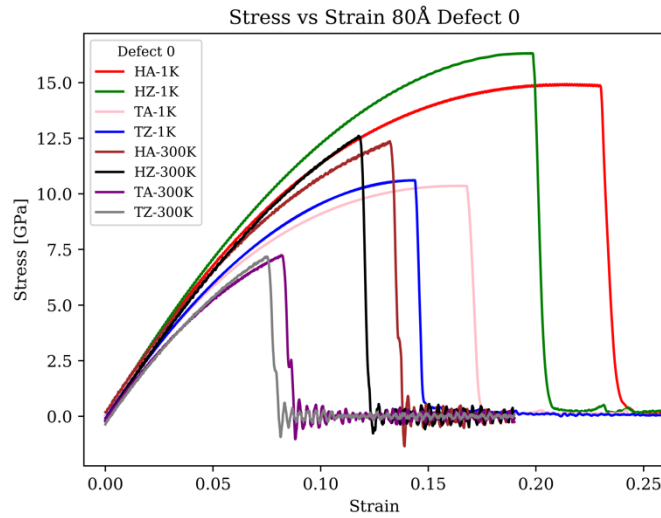


Fig. SM11. Stress-strain curves for defect-free MoS₂ nanotubes of 80 Å of diameter, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

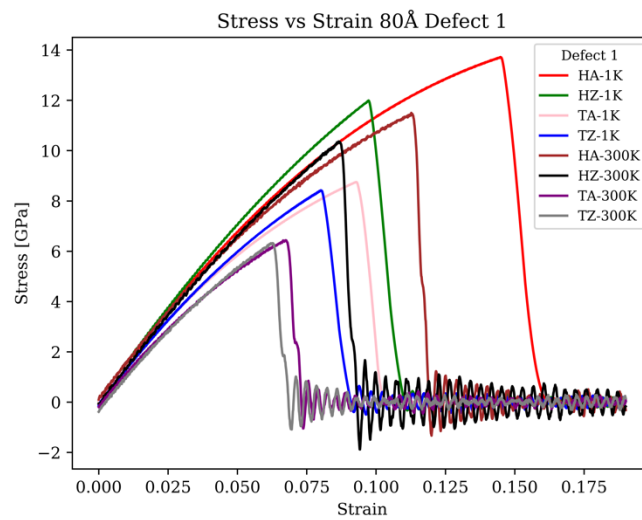


Fig. SM12. Stress-strain curves for MoS₂ nanotubes of 80 Å of diameter, with a defect of kind 1, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

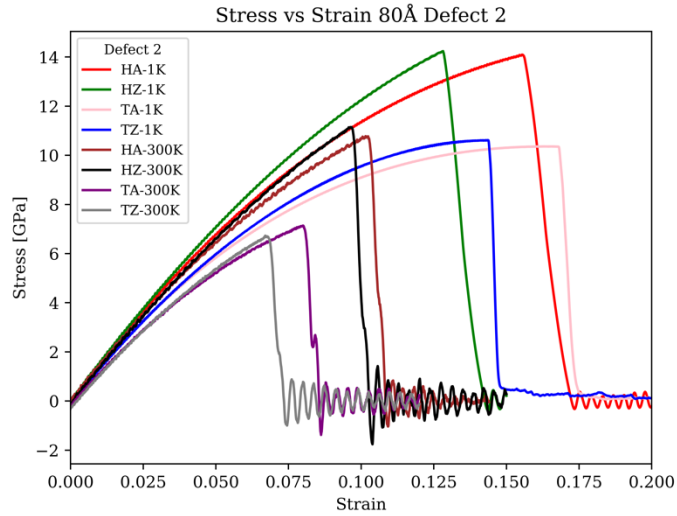


Fig. SM13. Stress-strain curves for MoS₂ nanotubes of 80 Å of diameter, with a defect of kind 2, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

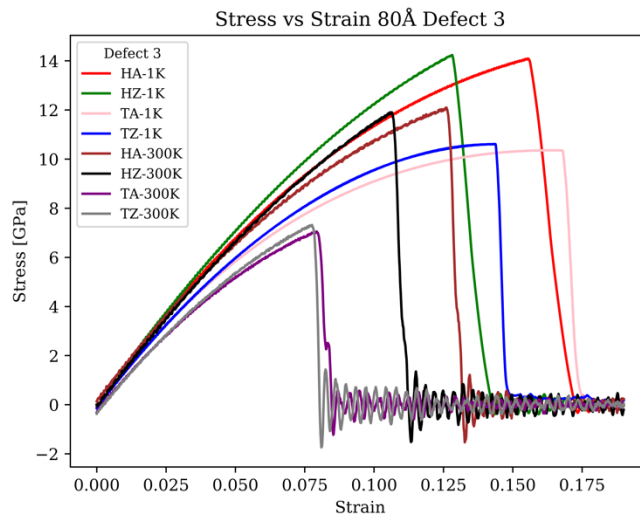


Fig. SM14. Stress-strain curves for MoS₂ nanotubes of 80 Å of diameter, with a defect of kind 3, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

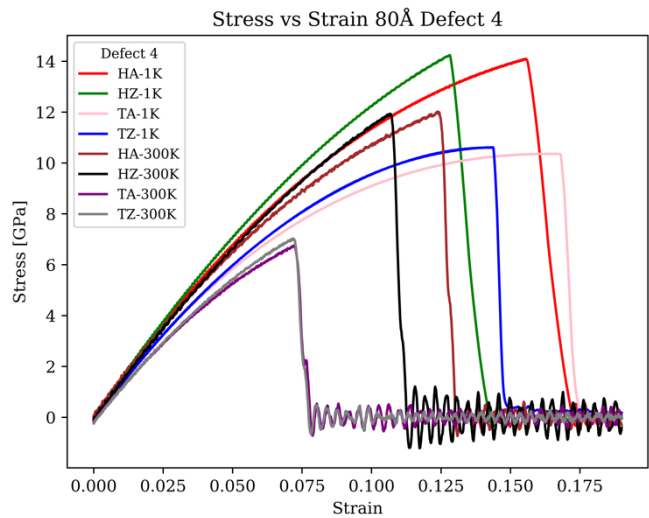


Fig. SM15. Stress-strain curves for MoS₂ nanotubes of 80 Å of diameter, with a defect of kind 4, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

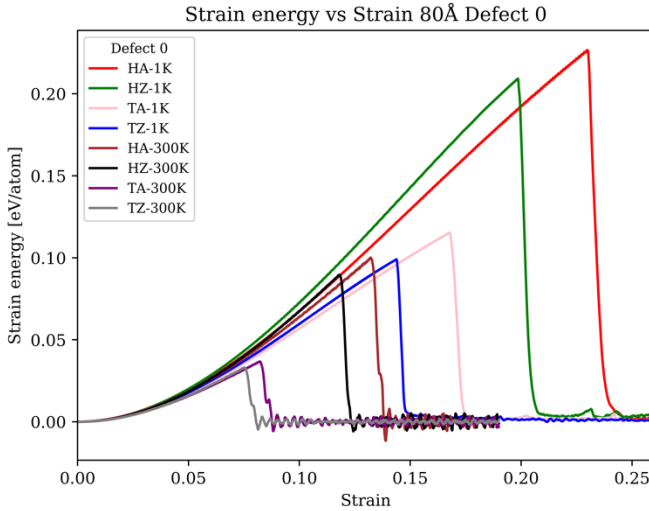


Fig. SM16. Strain energy vs strain curves for defect-free MoS₂ nanotubes of 80 Å of diameter, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

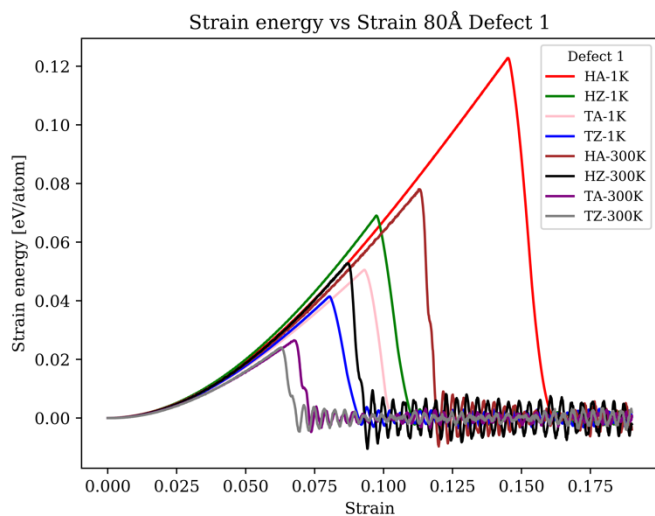


Fig. SM17. Strain energy vs strain curves for MoS₂ nanotubes of 80 Å of diameter, with a defect of kind 1, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

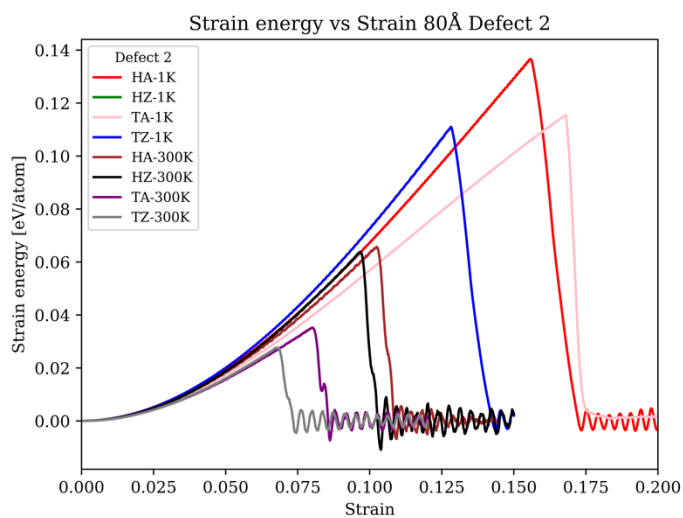


Fig. SM18. Strain energy vs strain curves for MoS₂ nanotubes of 80 Å of diameter, with a defect of kind 2, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

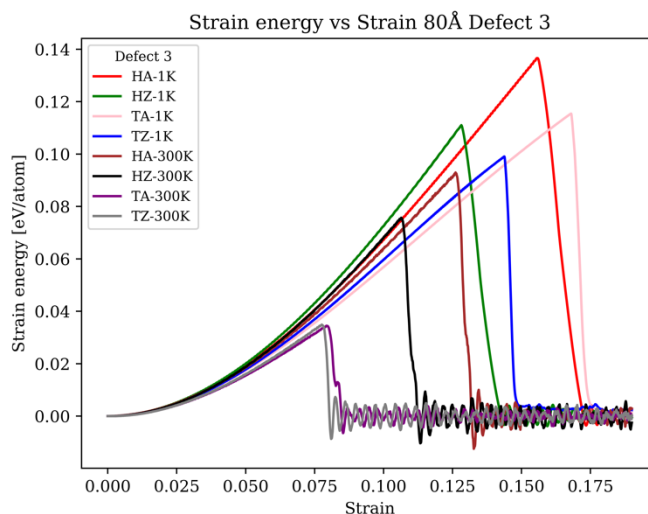


Fig. SM19. Strain energy vs strain curves for MoS₂ nanotubes of 80 Å of diameter, with a defect of kind 3, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

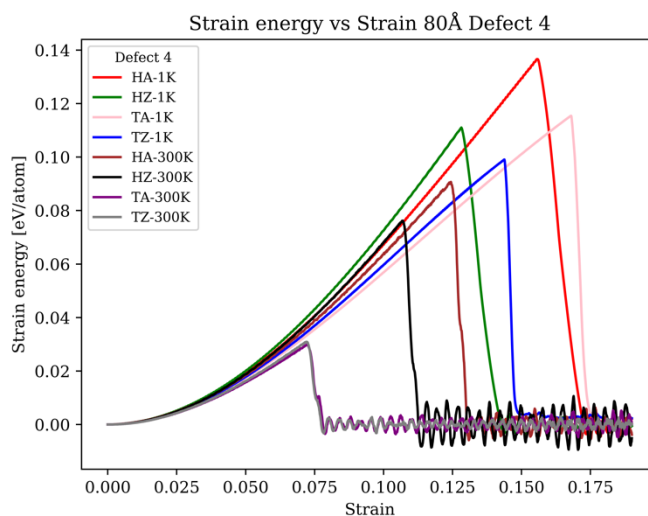


Fig. SM20. Strain energy vs strain curves for MoS₂ nanotubes of 80 Å of diameter, with a defect of kind 4, at 1 and 300 K. HA: Polytype H, armchair. HZ: Polytype H, zigzag. TA: Polytype T, armchair. TZ: Polytype T, zigzag.

II. Tensile strength and point of rupture vs Temperature for nanotubes of 60 Å of diameter

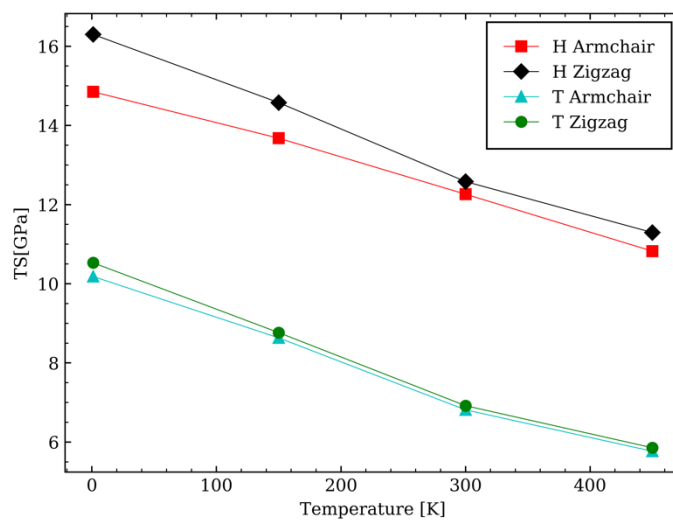


Fig. SM21. Young's modulus as function of temperature, for nanotubes of 60 Å of diameter.

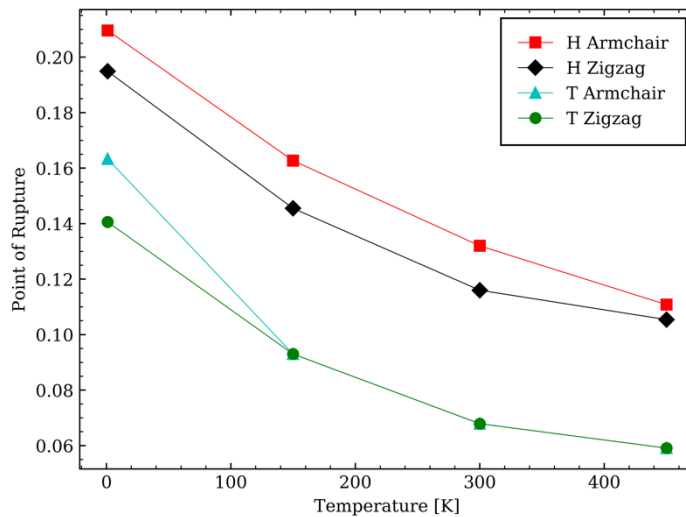


Fig. SM22. Point of rupture as function of temperature, for nanotubes of 60 Å of diameter.