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MD simulations of the tensile strength and failure mode of carbon nanotube junctions

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The tensile strength and failure mode of zigzag junctions are investigated under different strain rates, temperatures, and geometrical dimensions. Firstly, both the modified transition state theory (MTST) model and molecular dynamics (MD) simulations reveal that the yield strain of a junction depends linearly on the temperature and logarithmically on the strain rate. Moreover, MD simulations show that the yield strain is also affected by the curvature of the junction and the limit yield strain can be predicted by considering an unwrapped junction with the minimal curvature. Secondly, a junction may undergo a brittle or a ductile failure mode and the brittle-ductile transition (BDT) is dependent on the strain rate, temperature and geometrical dimension. The dominant geometrical factor affecting the failure modes is shown to be the aspect ratio rather than merely the diameter or length. Also, the BDT temperature, strain rate and aspect ratio is obtained.

Keywords: Tensile strength, Failure mode, Junction, MD simulations, Geometrical dimension.