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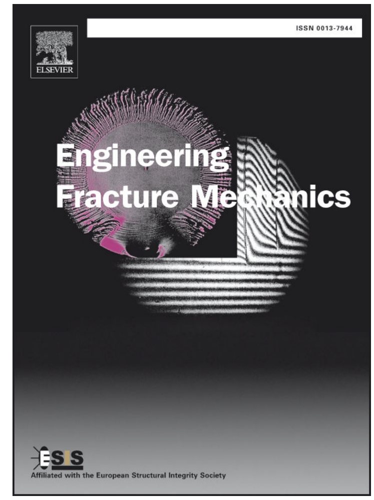

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Instability of rapidly accelerating rupture fronts in nanostrips of monolayer hexagonal boron nitride

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Abstract A molecular structural mechanics model of monolayer hexagonal boron nitride is constructed by finite element (FE) method, in which B-N bonds are equated with Timoshenko beam elements. Edge crack is introduced in nanostrip of FE model. Crack propagates straight and smoothly under pure opening displacement-loading, and crack speed reaches up to a stable value of 8.45 km/s finally at tensile loading rate 3.33 m/s of both upper and bottom boundaries. While crack branching or kinking occurs beyond critical speeds of 8.74 km/s and 8.71 km/s at higher loading rates of 16.67 m/s and 8.33 m/s respectively, with the formation of non-trivial crack surfaces. The above results are also examined by molecular dynamics models of the same sizes and geometry. Simultaneously, the critical energy release rate is equal to 0.136 TPa·Å at a critical tensile strain 8.27% with the occurrences of crack instabilities. Moreover, critical strains of crack initiation 5.75% and branching 8.27% are independent of displacement-loading rates.

Keywords Monolayer hexagonal boron nitride; Crack branching and kinking; Finite element; Molecular structural mechanics

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