

Accepted Manuscript

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PII: S0013-7944(18)30362-X

DOI: <https://doi.org/10.1016/j.engfracmech.2018.07.024>

Reference: EFM 6090

To appear in: *Engineering Fracture Mechanics*

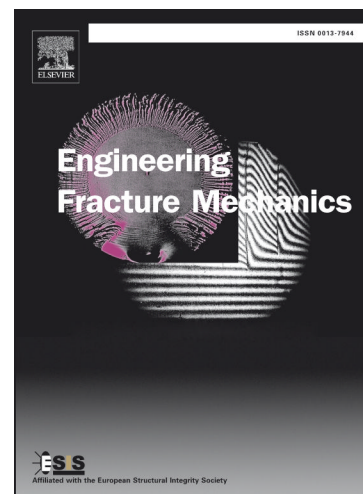
Received Date: 8 April 2018

Revised Date: 13 June 2018

Accepted Date: 14 July 2018

Please cite this article as: Tian, H., Yang, X., Yang, G., Zhang, B., Instability of rapidly accelerating rupture fronts in nanostrips of monolayer hexagonal boron nitride, *Engineering Fracture Mechanics* (2018), doi: <https://doi.org/10.1016/j.engfracmech.2018.07.024>

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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 $0.136 \text{ TPa} \cdot \text{\AA}$ 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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