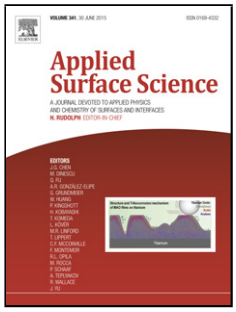

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Effects of twin boundaries in vanadium nitride films subjected to tensile/compressive deformations

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Highlights

- The effects of different twin boundary (TB) atoms and tension-compression asymmetry in VN are investigated.
- In compression, the migration of TBs with V atoms to that with N atoms contributes to softening.
- In tension, fractures occur at the TBs, which does not result in any improvement of fracture toughness and critical stress.
- Different deformation mechanisms are responsible for the plastic tension-compression asymmetry in VN.

Abstract: Two kinds of atoms can serve as the twin boundary (TB) atoms in a transition metal nitride (TMN). In this work, we performed molecular dynamics (MD) simulations for the responses of vanadium nitride (VN) films with different kinds of TB atoms (V or N) subjected to uniaxial tensile/compressive deformations, to investigate their effects and the tensile-compressive asymmetry. In compressive deformation, the migration of TBs with V atoms to that with N atoms contributes to softening, while the pile-up of dislocations at TBs contributes to strengthening. During tension, fractures occur at the TBs without distinct nucleation of dislocations, the nature of the brittle fracture, which does not result in any