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Nonlinear fracture of two-dimensional transition metal carbides (MXenes)

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ABSTRACT

As a newly discovered two-dimensional (2D) material group, MXene has exceptional thermal-electronic properties. However, its mechanical behavior, especially fracture, remains unexplored. In-situ SEM tensile experiments show that the fracture of MXene is quite nonlinear with a much-prolonged softening stage in comparison with other 2D materials, which is suspected to be caused by the anisotropy and relatively thick monolayer of MXenes. In this work, molecular dynamic (MD) modeling is conducted to investigate the anisotropic fracture behavior of two types of MXenes (Ti_2C and Ti_3C_2) with different monolayer thickness. Both pristine and defected MXenes are investigated. Results show that: (1) MXene tends to fracture along zigzag direction, (2) atomic vacancies at the crack tip have limited effects on the overall fracture behavior, (3) a thicker monolayer can produce a larger cohesive zone due to the 'thinning' process, (4) complex fracture paths are to be expected for mixed-mode fractures.

1. Introduction

Two-dimensional transition metal carbides (MXenes) have attracted great interest of the research community, as a relatively new and large class of 2D materials with unique electronic and optical properties [1–4]. Understanding the mechanical properties, especially fracture, is critical to application of MXenes in planar devices. Existing researches on fracture of 2D materials have focused on graphene and transition metal dichalcogenides (MoS_2 as an example) [5,6], which are often regarded as benchmarks.

At the atomic level, pristine graphene has a hexagonal lattice structure formed by strong covalent C-C bonds and reported to be one of the strongest materials with intrinsically brittle nature [7,8] as well as orientation dependence on mechanical and failure mechanisms [9,10]. Through *ab initio* calculation, Liu, F. et al. ascribe the intrinsically nature of brittle cleavage fracture for pristine graphene at low temperature to the longitudinal elastic wave nature of the soft phonon modes (or low-frequency temperature-dependent phonon modes [11]) when subjected to uniaxial tension [12]. Marianetti et al. confirmed this statement and further found that when loaded equi-biaxially, a mechanically unstable new phase will form due to the soft-mode phonon instability and leads to the fracture [13]. Additionally, loading along armchair direction creates a pure stretching scenario for highest-load bonds while loading along zigzag direction put the highest-load bonds under combination effect of bond stretching and rotation, leading to the anisotropy behavior [14]. Despite the theoretically high strength, results from in situ tensile testing [15] suggest a relatively low fracture toughness to the level of ideally brittle solid. In this manner, the inevitable flaws (atomic vacancies, crack-like defects for example) potentially lead to a significant strength loss at the macro-scale level [15–17]. Experimental and modeling studies showed that graphene could attain its high strength with few atomic vacancies and the influence of atomic vacancies increases with the

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