Abstract Submitted
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First-principles investigation on mechanical properties of ζ-Ta_4C_{3-x}[1] WEN-LI YAN, Beihang Univ, Univ of Utah, MICHAEL SYGNATOWICZ, DINISH SHETTY, Univ of Utah, GUANG-HONG LU, Beihang Univ, FENG LIU, Univ of Utah — As a group of transition metal carbides, tantalum carbides are of great interest due to their high melting temperature and high strength. Among different tantalum carbide phases of different space group and C/Ta atom ratio, the trigonal phase ζ-Ta_4C_{3-x} attracts special attention as high volume fraction of the ζ phase is reported to increase the fracture toughness of a tantalum carbide matrix. Using first-principles method, the structural and mechanical properties of ζ-Ta_4C_{3-x} have been investigated. The calculation results show that the weak bonding between Ta atoms in Ta_4C_3 is further weakened when structural vacancies occupy the carbon sub-lattice in ζ-Ta_4C_{3-x}. The (0 0 1) Ta surface is prominent to appear from surface energy and stacking fault energy calculations, consistent with the observed lamellar substructure during indentation process in fracture toughness measurements. The theoretical fracture toughness is derived from the Griffith relation, in comparison with the experimental results, to explain outstanding questions pertaining to mechanical properties of ζ-Ta_4C_{3-x}.

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