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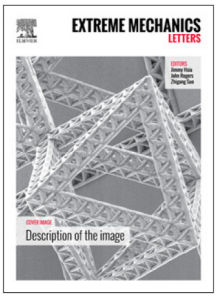

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The Role of Chemistry and Bonding in Regulating Fracture in Multiphase Transition Metal Carbides and Nitrides

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Abstract

The presence of the zeta phase in the tantalum carbides has been experimentally shown to give rise to very high fracture toughness which has been attributed to its complex microstructure. In this paper, electronic structure density functional theory is used to investigate the role chemistry and bonding play in regulating the fracture. These simulations demonstrate that fracture in the cubic carbide form is preferred along the {100} planes while the closed packed planes are preferred when carbon atoms are depleted from these planes. This is a consequence of the loss of all the primary covalent bonds across these planes, and idea that is rationalized using a broken-bond model. Thus, the fracture paths should follow the closed packed plane when carbon depleted stacking faults present in the zeta phase, and the {100} planes when they are not. Furthermore, our results demonstrate that these features are not unique to the tantalum carbides and are present in the vanadium carbides, niobium carbides and hafnium nitrides. This suggests that these materials may also have similar high fracture toughness's if the correct microstructure can be obtained through processing.

Keywords: carbides; ab initio; fracture

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