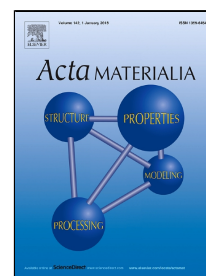


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Elastic properties and plastic deformation of TiC- and VC-based pseudobinary alloys

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Abstract

Transition-metal (TM) carbides are an important class of hard, protective coating materials; however, their brittleness often limits potential applications. We use density functional theory to investigate the possibility of improving ductility by forming pseudobinary cubic M^1M^2C alloys, for which $M^1 = \text{Ti}$ or V and $M^2 = \text{W}$ or Mo . The alloying elements are chosen based on previous results showing improved ductility of the corresponding pseudobinary nitride alloys with respect to their parent compounds. While commonly-used empirical criteria do not indicate enhanced ductility in the carbide alloys, calculated stress/strain curves along known slip systems, supported by electronic structure analyses, indicate ductile behavior for VMoC. As VMoC layers are sheared along the $\langle 1\bar{1}0 \rangle$ direction on $\{111\}$ planes, the stress initially increases linearly up to a yield point where the accumulated stress is partially dissipated. With further increase in strain, the stress increases again until fracture occurs. A similar mechanical behavior is observed for the corresponding TM nitride VMoN, known to be a ductile ceramic material.[1] Thus, our results show that VMoC is a TM carbide alloy which may be both hard and ductile, i.e. tough.

Keywords: Carbides, density functional theory, elastic properties, ductility, toughness

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