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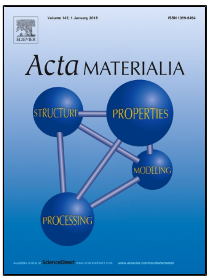

Elastic properties and plastic deformation of TiC- and VC-based pseudobinary alloys

D. Edström, D.G. Sangiovanni, L. Hultman, Ivan Petrov, J.E. Greene, V. Chirita

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

D. Edström,[1,*] D. G. Sangiovanni,[1,2] L. Hultman,[1] Ivan Petrov,[1,3] J. E. Greene,[1,3] and V. Chirita[1]

[1]Department of Physics, Chemistry, and Biology (IFM)
Linköping University, SE-58183 Linköping, Sweden

[2]ICAMS, Ruhr-Universität Bochum, D-44801 Bochum, Germany

[3]Frederick Seitz Materials Research Laboratory and the Materials Science Department, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA

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 = Ti or V and M^2 = 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

[*]**Corresponding author**: Daniel Edström, Tel. 0046 13286693, Fax 0046 13137568 , daned@ifm.liu.se