

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Design of carbide thin film coatings from first principles MIKAEL RÅSANDER, University of California Davis, BIPLAB SANYAL, ULF JANSSON, OLLE ERIKSSON, Uppsala University — Transition metal carbides have many interesting physical properties and have therefore been used in many technological applications, e.g. as thin film metal coatings. A commonly studied thin film coating material is nc-TiC/a-C, where nanocomposites (nc-) of TiC are dispersed in an amorphous (a-) C matrix. An interesting feature of these types of materials is the possibility to design the material to obtain new functionality, e.g. by tuning the C to Ti content. In this talk we will present results obtained by first principles density functional theory calculations of a different approach, where various metals have been alloyed into TiC. Depending on the alloying metals ability to form carbides this will yield different effects. One of these effects is the creation of a driving force for the release of C from the carbide. This C release has been shown to yield favorable lubricating properties of nc-(Ti,Al)C/a-C thin films. We will show that the C release can be tuned by a careful selection of the alloying metal in order to optimize the properties of these types of thin film carbide coatings.

Mikael Rålander
University of California Davis

Date submitted: 19 Nov 2010

Electronic form version 1.4