Carbon sweating of meta-stable ternary carbides

MIKAEL RÅSANDER, Uppsala University, ERIK LEWIN, BIPLAB SANYAL, MATTIAS KLINTENBERG, ULF JANSSON, OLLE ERIKSSON — Transition metal carbides (TMC) have many attractive and unique physical properties and are nowadays used regularly in many technological applications. In thin films, the TMC can form nanocomposites where nanocrystallites of the carbide are embedded in a carbon matrix. Here we report on a new development where we have investigated meta-stable nanocomposite TMC. By substitutionally dissolving a weak carbide forming metal into a stable monocarbide, the ternary carbide system will become meta-stable and a decomposition into more stable phases will occur. We will show results obtained by density functional theory calculations of meta-stable TMC, where we have alloyed the stable monocarbide TiC with elements from the 3d transition metal series. The stability of the alloyed ternary phase decreases with the amount of alloying metal, which creates a driving force for the release of carbon from the carbide, i.e. the carbide sweats carbon. This mechanism can be controlled by careful tuning of the amount and selection of the alloying metal. These findings are supported by experimental studies on thin films of nanocomposite TMC.