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Role of defects and impurities on the thermal stability of transition-metal nitrides and carbides L. TSETSERIS, N. KALFAGIANNIS, S. LOGOTHETIDIS, Aristotle University of Thessaloniki, Thessaloniki, Greece, S. T. PANTELIDES, Vanderbilt University, Nashville, TN — Transition-metal nitrides and carbides are used in a variety of applications because of their renowned hardness and stability. Here, we present the results of first-principles calculations on point defects and impurities in the prototype systems of TiN and TiC, and in HfN and ZrN. We find features which are common to all systems, while we unravel also key differences. In cases, for example N interstitials in TiN, the interaction between defects is attractive and it favors the formation of defect complexes. Moreover, we show that the atomic-scale mechanisms of interaction and migration of point defects and their complexes can account for various changes of transition metal nitrides and carbides after annealing at widely different temperatures. Finally, we discuss the fundamentals of trapping and release of the most common impurities in TiN. The work was supported in part by the McMinn Endowment at Vanderbilt University, AFOSR MURI Grant FA9550-05-1-0306, and GSRT-PENED- 03ED613.

Leonidas Tsetseris
Aristotle University of Thessaloniki, Thessaloniki, Greece

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