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Role of Interfaces and Effect of Impurities in Nitride-based Superhard Nanocomposites HAO SHIQIANG, The University of Sydney, BERNARD DELLEY, Paul-Scherrer-Institut, CATHERINE STAMPFL, The University of Sydney — Recently, a hardness similar to that of diamond has been reported for the ternary nitride-based nanocomposite, *nc*-TiN/ *a*-Si_3N_4/*a*- and *nc*-$TiSi_2$ [1]. The reproducibility, however, has proved difficult, as has the superhardness of the related, prototypical, binary nanocomposite *nc*-TiN/*a*-Si_3N_4. Extensive density- functional theory calculations indicate that the hardness enhancement in the latter system is due to the preferential formation of TiN(111) polar interfaces with a thin Si-layer which is N-coordinated and tetrahedrally bonded [2]. The tensile strength of TiN in the [111] direction is very similar to the weakest bonding direction in diamond. Oxygen impurities cause a significant reduction of the interface strength which could partly explain the conflicting results, and signals the importance of avoiding such contaminants for achieving super- and ultra-hard nanocomposites.
[1] S. Veprek et al. Surf. Coat. Technol. 133-134, 152 (2000).
[2] S. Hao, B. Delley, and C. Stampfl, to be published.

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