

Abstract Submitted
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First-Principles Calculations for the Dislocations in Titanium Nitride¹ RAMKUMAR GUDIPATI, University of Tulsa, Y.G. SHEN, City University of Hong Kong, WENTAO XU, University of Kentucky, A.S. RAO, H.L. DANG, SANWU WANG, University of Tulsa — Nanostructuredsuperhard materials have been successfully synthesized in recent years. The hardness of nanosuperlatticesand nanocomposites significantly exceeds that of the component materials. While it is believed that the nanodimensions are needed to impede dislocation activity and grain-boundary sliding, relevant calculations are rare. We report first-principles density-functional calculations for the core structures and energetics of various dislocations including the $[110]\{110\}$, $[110]\{111\}$, $[110]\{100\}$, $[100]\{100\}$ and $[100]\{110\}$ edge dislocations in bulk TiN. We found that the formation energies of the core dislocations were continuously increased when their sizes decreased. We also found that the most common types of dislocations in TiN are the $[110]\{110\}$ and $[110]\{111\}$ edge dislocations. The obtained results are helpful for elucidating the atomic-scale mechanism for the superhardness of nanocomposites.

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Ramkumar Gudipati
University of Tulsa

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