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First-principles calculations for the elastic properties of super-hard TiN/Si₃N₄ superlattices¹ SANWU WANG, Department of Physics and Engineering Physics, University of Tulsa, Tulsa, OK 74104, Y.G. SHEN, Department of Manufacturing Engineering and Engineering Management, City University of Hong Kong, Hong Kong, S.T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235 — We report first-principles density-functional calculations for the atomic structures, the electronic properties, and the elastic properties of superlattices containing nano-scale crystalline TiN and thin layer of silicon nitride. We found that the elastic properties (bulk modulus, shear modulus, and elastic constants) are strongly dependent on the size of the components. Superlattices with TiN thickness smaller than 2.5 nm have far smaller values of bulk and shear moduli than bulk crystalline TiN, while ~3 nm TiN can make the superlattice have the elastic properties close to those of crystalline TiN. The results are helpful for optimization of the component size to achieve high values of both elastic properties and hardness.

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