First-principles study of superhard SiN_x /TiN nanocomposites

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Nanocomposite materials based on TiN nanocrystalites embedded in an amorphous silicon nitride matrix with thickness of only a few atomic layers and composition close to Si_3N_4 show a superhardness similar to that of diamond. To elucidate the chemical origin of the material hardness and the exceptional strength of the SiN_x /TiN interfaces we have used DFT calculations in combination with Car-Parrinello molecular dynamics (CPMD) simulations to create and to investigate model SiN_x /TiN interface structures. As the first step we studied the initial stages of SiN_x layer formation on TiN(001) by adding successively silicon and nitrogen atoms to the TiN surface to form up to two monolayer thick SiN_x films with different composition. For a selected set of configurations, chosen on the basis of thermodynamic stability, we then applied a stepwise procedure based on heating, quenching and final geometry optimization to search for stable and energetically favorable amorphous structures of SiN_x films and stacks of SiN_x /TiN multilayers. The relative stability of the different model interface structures is analyzed in terms of Ti, Si and N coordination numbers, and the mechanical strength of the interfaces is assessed by the calculation of stress–strain curves to determine the ideal decohesion strength.