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Bond Angles in the Crystalline Silicon/Silicon Nitride Interface

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— Silicon nitride deposited on a silicon substrate has major applications in both dielectric layers in microelectronics and as antireflection and passivation coatings in photovoltaic applications. Molecular dynamic simulations are performed to investigate the influence of temperature and rate of externally applied strain on the structural and mechanical properties of the silicon/silicon nitride interface. Bond-angles between various atom types in the system are used to find and understand more about the mechanisms leading to the failure of the crystal. Ideally in crystalline silicon nitride, bond angles of 109.5 ° occur when a silicon atom is at the vertex and 120 ° angles occur when a nitrogen atom is at the vertex. The comparison of the calculated angles to the ideal values give information on the mechanisms of failure in silicon/silicon nitride system.

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