

Abstract Submitted
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Pair distribution functions of silicon/silicon nitride interfaces¹

DENG CAO, MARTINA E. BACHLECHNER, West Virginia University, Physics Department — Using molecular dynamics simulations, we investigate different mechanical and structural properties of the silicon/silicon nitride interface. One way to characterize the structure as tensile strain is applied parallel to the interface is to calculate pair distribution functions for specific atom types. The pair distribution function gives the probability of finding a pair of atoms a distance r_{apart} , relative to the probability expected for a completely random distribution at the same density. The pair distribution functions for bulk silicon nitride reflect the fracture of the silicon nitride film at about 8 % and the fact that the centerpiece of the silicon nitride film returns to its original structure after fracture. The pair distribution functions for interface silicon atoms reveal the formation of bonds for originally unbound atom pairs, which is indicative of the interstitial-vacancy defect that causes failure in silicon.

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