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Spatial Stratification of Order As Used in Failure Analysis¹ ROBERT H. LEONARD, MARTINA E. BACHLECHNER, Physics Department, West Virginia University — Silicon nitride deposited on silicon substrates has application in dielectric layers for microelectronics as well as in photovoltaics. During production and operation of components involving silicon/silicon nitride interfaces, stresses and strains can build up at various temperatures resulting in component failure. Using molecular dynamics simulations the influence of temperature and rate of externally applied strain on silicon/silicon nitride interfaces has been analyzed. The primary purpose of this research is to understand the mechanisms leading to the failure of these films. Analyses involving bond lengths and angles have been developed to gain insight into these mechanisms. Methods for stratifying bond lengths and bond angles into unique sub-populations on the basis of spatial orientation have been developed, and have given much insight to how the material behaves, particularly with regards to the Poisson effect. Possible extensions of this stratification method to primitive rings will also be examined. In combination with experimental observations, this analysis will deepen our understanding of the structural properties of silicon/silicon nitride interfaces.

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