Abstract Submitted
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Molecular Dynamics Simulations of Interface Failure[1] MARTINA E. BACHLECHNER, Physics Department, West Virginia University, DENG CAO, ROBERT H. LEONARD, ELI T. OWENS, WM. TREVOR SWAN, III, SAMUEL C. DUCATMAN[2], Physics Department, West Virginia University — The mechanical integrity of silicon/silicon nitride interfaces is of great importance in their applications in micro electronics and solar cells. Large-scale molecular dynamics simulations are an excellent tool to study mechanical and structural failure of interfaces subjected to externally applied stresses and strains. When pulling the system parallel to the interface, cracks in silicon nitride and slip and pit formation in silicon are typical failure mechanisms. Hypervelocity impact perpendicular to the interface plane leads to structural transformation and delamination at the interface. Influence of system temperature, strain rate, impact velocity, and system size on type and characteristics of failure will be discussed.

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