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Density of Surface States in a-Si/Ge Using a Two Parameter Hamiltonian ELIEZER RICHMOND, Retired — To rigorously investigate the contribution of surfaces to the density of electronic states of a-Si/Ge and the effect of the topology on the density of surface states (DOS), a surface for amorphous homopolar tetrahedral solids is defined. The density of unsaturated bonds is 0.106 bonds/Å^2. Reconstruction enables a 88% reduction in the density of unsaturated bonds. The effects on the DOS in the valence band and energy gap is investigated using a two parameter Hamiltonian. The local and configuration DOS are computed for the unsaturated bond and the four back bond hybrids. The ring structure effects the DOS in the valence band, but not the more localized energy gap states. The spectral feature due to surface atoms with only one unsaturated bond is affected by the topology. The antibonding spectral feature in the energy gap deriving from surface atoms with 2 or 3 unsaturated bonds is independent of all topological effects while the bonding spectral feature from these same surface atoms is not. Comparison with empirical results verifies the contribution of the unsaturated bonds to ESR signals and elucidates the origin of the subtle valence band features in UPS spectra.

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