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Density of Surface States in the Region of the Energy Gap for 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 (DOSS), a surface for amorphous homopolar tetrahedral solids has been defined.[1] The effects on the DOSS in the region of the energy gap are investigated using a two parameter Hamiltonian. We address the effects of ring structure, nearest neighbor dangling bonds, multiple dangling bonds per surface atom, and back bonds on the DOSS. In particular, the results here predict a shift of 0.12 eV of the bulk p-like peak at the top of the valence band to higher energies due to the DOSS. Additionally, surface contributions in the lower portion of the conduction band (CB) give rise to a hump in the lower portion of the CB density of states. Lastly, a gap state is found 0.6 eV below the CB edge. These conclusions will be compared to experimental results and are found to be in surprisingly good agreement.

[1]http://www.tandfonline.com/eprint/dZXIzBKDCsZVENFurTZs/full

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