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Microstructural properties of hydrogenated amorphous silicon: A first-principles study[1] DURGA PAUDEL, PARTHAPRATIM BISWAS, The University of Southern Mississippi, RAYMOND ATT-FYNN, University of Texas,Arlington,TX, DAVID DRABOLD, Ohio University, Athens Ohio, STEPHEN ELLIOTT, University of Cambridge,UK — We present a new approach to simulate complex amorphous materials with an emphasis on structural, electronic, and optical properties of hydrogenated amorphous silicon. The microstructural properties of hydrogen distribution are addressed by simulating very large models using a method that combines classical metadynamics simulations with density-functional calculations. The shape, size and distribution of microvoids and their number density are studied and compared with the same from the small-angle X-ray scattering, hydrogen- and helium-effusion measurements, and neutron diffraction studies on *a*-Si:H. Our results suggest that the density of microvoids is of the order of 7-8 $\times 10^{18}$ cm^{-3} for device-quality models with 8-10 at. % H, and it increases to 2-3 $\times 10^{19}$ cm^{-3} for concentration of up to 18 at. %. The geometry of the microvoids has been found to be highly complex with a radius of gyration from 2.8 Å to 4.0 Å for very large models.

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