

Hydrogenated amorphous Si (α -Si:H) has seen a renewed interest for its application in heterojunction with intrinsic thin-layer (HIT) solar cells. Known deficiencies in this material's photovoltaic properties are limited hole mobilities and the Staebler-Wronski effect, a light-induced degradation of efficiency which may be in part due to voids within the structure. Simulations of voids in α -Si typically involve atomic removal, but these methods require an a priori idea of the bonding structure near the void. Instead, we generate voids within α -Si and α -Si:H using a fast, unbiased approach: the Wooten-Winer-Weaire classical-potential Monte Carlo method where we vary the density and replace some Si-Si bonds with Si-H bonds. At low density, voids form (like cavitation in a liquid), maintaining 4-coordination but increasing bond angle deviation, reducing medium-range order, and altering local structure within 4 Å of the void. This work provides a set of void structures for further studies of their effects on degradation, hole mobility, two-level systems, thermal transport, and elastic properties. (E. Guerrero and D. A. Strubbe Phys. Rev. Materials **4**, 025601 (2020))