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What happens to the energy of recrystallization of amorphous Si?

J.A. VAN VECHTEN, EECS Oregon State University — Si ICs require annealing a-Si to regain x-Si without nucleating crystallites ahead of the recrystallization front. Accepted models of a-Si (Gilmer et al. 2001) describe the state as a dense array of "I-V pairs," linked 5 and 7 member rings that can revert to x-Si by a rebonding and small motion of 2 neighboring atoms to make 6 member rings. The defect energy is $\sim$ 3.5 eV, enough to melt between 6 and 7 x-Si atoms if it were abruptly delivered into the small region where the 2 odd rings intersect. Explosive crystallization of crystallites would be expected where 1 defect reverted in the a-Si. If the 2 atoms of the defect were to revert according to a configuration coordinate model like that of the Glyde-Flynn model of atomic diffusion, the energy would be abruptly deposited where the rings intersect by the atoms coming down from the saddle point. An alternative that would avoid the local release of atomic kinetic energy would be for the constraining bonds of the 2 odd rings to be momentarily weakened by an accumulation of h+s and e-s in localized bonding and antibonding states about the defect intersection long enough for the rebonding and motion of the 2 atoms to occur with little kinetic energy. To explain why this happens at steps on the recrystallization front and not in the bulk of the a-Si, one concludes that the localized states are confined to steps than in the bulk.

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