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The stability of vacancy-like defects in amorphous silicon JEAN-FRANCOIS JOLY, NORMAND MOUSSEAU, Universite de Montreal — The contribution of vacancy-like defects to the relaxation of amorphous silicon (a-Si) has been a matter of debate for a long time. Due to their disordered nature, there is a large number local environments in which such a defect can exists. Previous numerical studies the vacancy in a-Si have been limited to small systems and very short timescales. Here we use kinectic ART (k-ART), an off-lattice kinetic Monte-Carlo simulation method with on-the-fly catalog building [1,2] to study the time evolution of 1000 different single vacancy configurations in a well-relaxed a-Si model. Our results show that most of the vacancies are annihlated quickly. In fact, while 16% of the 1000 isolated vacancies survive for more than 1 ns of simulated time, 0.043% remain after 1 ms and only 6 of them survive longer than 0.1 second. Diffusion of the full vacancy is only seen in 19% of the configurations and diffusion usually leads directly to the annihilation of the defect. The actual annihilation event, in which one of the defective atoms fills the vacancy, is usually similar in all the configurations but local bonding environment heavily influence its activation barrier and relaxation energy.

[1] El-Mellouhi et al,Phys. Rev B. 78, (2008)
[2] Beland et al., Phys. Rev. E. 84, (2011)

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