Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Accelerated kinetics of amorphous silicon using an on-the-fly off-lattice kinetic Monte-Carlo method JEAN-FRANCOIS JOLY, Universite de Montreal, FEDWA EL-MELLOUHI, Texas A&M University at Qatar, LAURENT KARIM BELAND, NORMAND MOUSSEAU, Universite de Montreal — The time evolution of a series of well relaxed amorphous silicon models was simulated using the kinetic Activation-RelaxationTechnique (kART), an on-the-fly off-lattice kinetic Monte Carlo method [1]. This novel algorithm uses the ART nouveau algorithm to generate activated events and links them with local topologies. It was shown to work well for crystals with few defects but this is the first time it is used to study an amorphous material. A parallel implementation allows us to increase the speed of the event generation phase. After each KMC step, new searches are initiated for each new topology encountered. Well relaxed amorphous silicon models of 1000 atoms described by a modified version of the empirical Stillinger-Weber potential [2] were used as a starting point for the simulations. Initial results show that the method is faster by orders of magnitude compared to conventional MD simulations up to temperatures of 500 K. Vacancy-type defects were also introduced in this system and their stability and lifetimes are calculated.

[1] El-Mellouhi et al., ,Phys Rev. B, 78, 153202 (2008)
[2] Vink et al., J. Non-Cryst. Sol. 282, 248 (2001)

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Date submitted: 18 Nov 2010 Electronic form version 1.4