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Energy gain by defect formation: a new tight binding annealed model for a-Si JOSEPH FELDMAN, Naval Research Laboratory and George Mason University, NOAM BERNSTEIN, Naval Research Laboratory, MARCO FORNARI, Central Michigan University, DIMITRIS PAPACONSTANTOPOULOS, Naval Research Laboratory and George Mason University — We have obtained a new structure of a-Si by annealing with QM forces a Wooten CRN type 216 model. The annealing was done for 1.2 ns (1.2 million time steps) and the NRL tight binding method was employed. We obtain the total energy, electronic density of states, and force constants of the model. Whereas the starting model had no coordination defects several were present in the final model. As expected these defects were found to give rise to states in the gap as determined both by charge self-consistent TB calculations and DFT (pseudopotential) calculations, where the latter were performed on related "relaxed" models within DFT. The final model was of lower total energy than the starting model, both within the TB method and within the psedopotential method. The normal mode properties based on our force constant determination within TB will also be discussed.

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