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A Kinetic Monte Carlo Model for Material Aging: Simulations of Second Phase Formation at Au/Bi_2Te_3 Junction in Oxygen Environments

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ABSTRACT

Properties of semiconductor devices are sensitive to second phase precipitates, grain sizes, and voids. These defects evolve over time especially under oxidation environments. In this paper, we develop a kinetic Monte Carlo framework aiming at simultaneous simulation of the evolution of second phases, precipitates, grain sizes, and voids in complicated systems involving many species including oxygen. As a first step of our model implementation, we incorporate the second phase formation module in the parallel kinetic Monte Carlo codes SPPARKS. Selected aging simulations are performed to examine the formation of second phase precipitates at the interface of Au/Bi_2Te_3 multilayers under oxygen-containing and oxygen-free environments, and the results are compared with the corresponding experiments.

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