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New Indexing Method for Zinc Blende Crystals: Applied to Kinetic Monte Carlo Simulations[1] KYLE BENTLEY, RYOICHI KAWAI, Univ of Alabama - Birmingham — Usual methods of indexing a zinc blende, or diamond cubic lattice with Cartesian coordinates is cumbersome to use in Monte Carlo simulations with fixed-length step sizes. There is to date no method of quickly gathering information about specific neighboring atoms that isn't costly in terms of computational time. We have shown that a simplified method of indexing a zinc blende and diamond cubic lattice can reduce the complexity of simulations, while at the same time increase computational performance. These methods prove useful in modeling the diffusion of native defects and dopants in binary compound systems, such as chalcogenide, oxide, and nitride systems, as well as diamond, silicon, germanium, and many others. Utilizing these algorithms we are able to simulate diffusion time scales in the microsecond regime in a reasonable amount of time. We will show kinetic Monte Carlo simulations of diffusion in zinc oxide crystals.

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