Monte Carlo simulations 2006. Exercise 6

To be handed in Thu Apr 13, solutions given Tue Apr 18 10:15.

1. (40 p) A self-interstitial atom is an extra atom in a crystal lattice, of the same type as the ordinary lattice atoms. A vacancy is a lattice site where an atom is missing.

Consider interstitials (i) and vacancies (v) in silicon. Their mobility can be expressed as

$$\text{jump rate(T)} = we^{-E^m/k_BT}$$

where w is the jump rate prefactor and E^m the migration activation energy. According to a recent theoretical paper [Tang, Phys. Rev. B. 55 (1997) 14279],

$$\begin{aligned} w_i &= 1.717 \text{ 1/fs} \\ E_i^m &= 1.37 \text{ eV} \\ w_v &= 0.001282 \text{ 1/fs} \\ E_v^m &= 0.1 \text{ eV} \end{aligned}$$

In kinetic Monte Carlo simulations, it is common practice to describe defect motion in Si as if it would occur in a random medium (so you can ignore the lattice structure). The jump distance is nevertheless set to the nearest-neighbour distance in Si, 2.35 Å. In addition to moving at the rates described above, the i and v have the property that if they come to within $r_{\text{recombine}} = 4.0$ Å from each other, they spontaneously recombine and hence vanish completely. For this exercise, we further assume no other defect reactions exist (in reality defect clustering plays an important role).

Consider now a radioactive impurity which decays deep inside perfect crystalline Si. If it has a high recoil energy, it will produce vacancies and interstitials. As a crude first approximation, we can assume that this kind of an event will produce 150 interstitials and 150 vacancies. Because of the nature of the collisional processes, the defects are distributed such that the interstitials are farther out from the center than the vacancies. Let us again do a crude (but qualitatively not too bad) approximation that the defects are both distributed randomly around the center with a Gaussian probability distribution describing the r dependence, and uniformly in θ and ϕ. The standard deviation of the Gaussian is $r_v^d = 20$ Å for vacancies and $r_i^d = 60$ Å for interstitials.

Write a KMC code which produces this kind of defect distribution, and simulates what happens with the defects until a time of 1 μs.

Examine the system at the temperatures 500, 1500, and 2500 K, and describe the behaviour qualitatively. For each temperature, report the a) average fraction of surviving defects, and b) the ratio of interstitial jumps compared to vacancy jumps.

Also calculate a statistical uncertainty for all the quantities (you are allowed to get the uncertainty simply by repeating runs a few times and calculate the erros assuming Gaussian statistics).

c) Can you explain why the fraction of surviving defects is relatively independent of temperature?

d) Repeat the simulations at 1500 K using $r_{\mathrm{recombine}} = 10.0$ Å, and determine again the average fraction of surviving defects with uncertainties. Comment on the difference.

Return the code.