Simulation of effective atomic movements of substitutional impurities in cs, fcc and bcc lattices using a random walk algorithm

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From a "macroscopic" point of view, material composition is assumed to vary smoothly along its microstructure. A closer look reveals that, at the atomic level, the material composition does not change so smoothly. Single atoms jump randomly along the crystal lattice due to their thermal energy. These random jumps create sporadic zones of the crystal with higher concentration of certain elements, and they are responsible for many phenomena, such as spinodal decomposition, segregation, precipitation, Ostwald ripening… This work obtains some useful relations between atomic jumping rate and macroscopic diffusivity, for substitutional impurities in simple cubic, face-centred cubic and body-centred cubic atomic lattices.

To simulate the diffusion of these impurities a random walk based parallel code was developed. This code handles two main elements, individual lattice cells and individual atoms. From the point of view of cells, the program knows the position of all system cells and their amount of impurities. From the point of view of atoms the code knows the position of each atom, via the cell that it belongs to. To simulate the diffusion, the program moves sequentially all impurities present in the system. On each diffusion step, each impurity is swapped with one of its nearest neighbours. The neighbour used for each swap is randomly chosen for each diffusion step and for each impurity [1].

Due to the fluctuations of the composition at atomic scale results obtained with the model are very noisy. In order to obtain statistically significant results we simulate systems with a huge number of atomic cells, to average the random nature of the model. Results shown in this work were obtained simulating a 1000×1000×1000 cells microstructure. To avoid border effects, periodical boundary conditions were applied to these microstructures [2].

A set of simulations was performed to obtain the relation between the macroscopic diffusivity and the atomic jumping frequency. The simulated microstructure consists on a prism initially divided in two halves, one of them without any impurity and the other one with an initial concentration of impurities of 100 ppm. These impurities are randomly placed within the second half of the prism. Once the initial microstructure is generated, atoms are allowed to jump. The evolution of the simulated concentration profile is compared, after each diffusion step, with the profile obtained analytically for a known diffusivity and for a fixed time [3]. From the diffusion steps needed to match the analytical profile it is possible to determine the atomic jumping frequency that corresponding to that diffusivity. Figure 1 shows the results for the atomic jumping frequency obtained for 3 different atomic lattices; simple cubic, body-centred cubic and face-centred cubic, with a lattice parameter of 1 nm.

From analytical-continuum results, and assuming that jumping frequency, Γ, is proportional to the diffusivity, *D*, it is possible to obtain the relation between the jumping frequency and the crystallographic cell size, *a*. Relations shown in equation 1 were obtained by matching simulations with these analytical calculations.

$$\begin{aligned} \Gamma_{cs} &= 5.91\, D / a^2 \\ \Gamma_{bcc} &= 3.93\, D / a^2 \\ \Gamma_{fcc} &= 6.17\, D / a^2 \end{aligned} \qquad (1)$$

Only the simple cubic case agrees with the Einstein's Formula [4]. For the other two cases, the number of nearest neighbours, 8 and 12 for bcc and fcc cases respectively, and the distance between atoms, $\lambda_{bcc}=\sqrt{3}/2$ and $\lambda_{fcc}=\sqrt{2}/2$, do not make possible this agreement.

From the results obtained in this work it is possible to obtain, from the macroscopic diffusivity, the atomic jumping frequency needed to simulate the diffusion of substitutional impurities in cs, bcc and fcc lattices.

References:

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Figures:

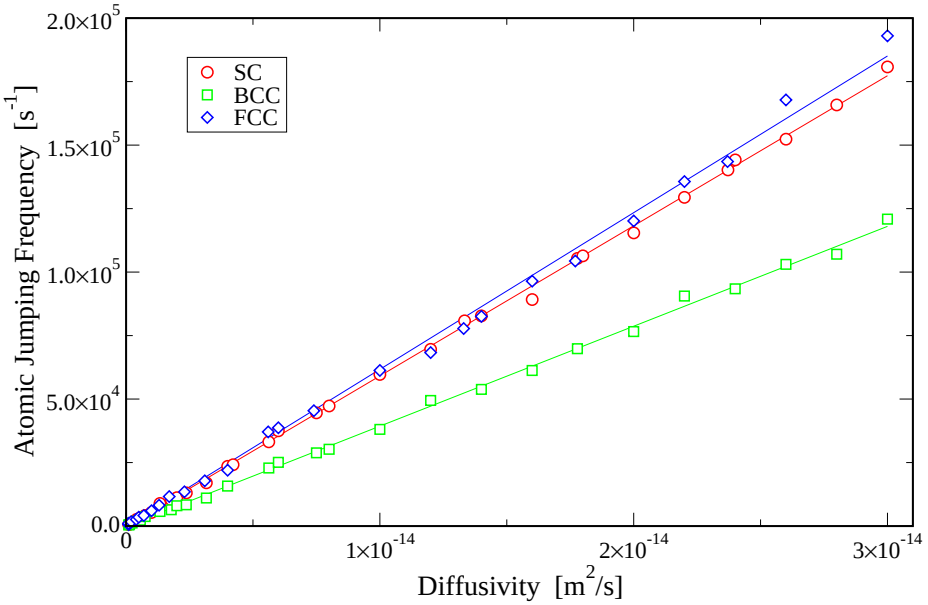

Figure 1: Atomic jumping frequencies needed to simulate different diffusivities for SC, BCC and FCC lattices, for a cell size of 1 nm.