Exercice 2 - Diffusion Vacancies

In this exercice we will implement a system in which the activation energy of an event change as function of environment. This situation can be associate to system of spin, alloy or diffusion vacancies in a solid for instance. Basically you are 2 or more state of site in the system and we take into account the interation between the neighbors site. The interaction between two sites in the same state is different to the interaction between two differents sites. To illlustrate this situation we show in figure 1 an asymetric barrier between two local minimum. In this case we will have two differents activation energies $E^1_{ac} = E_{ac}$ and $E^2_{ac} = E_{ac} - dE$.

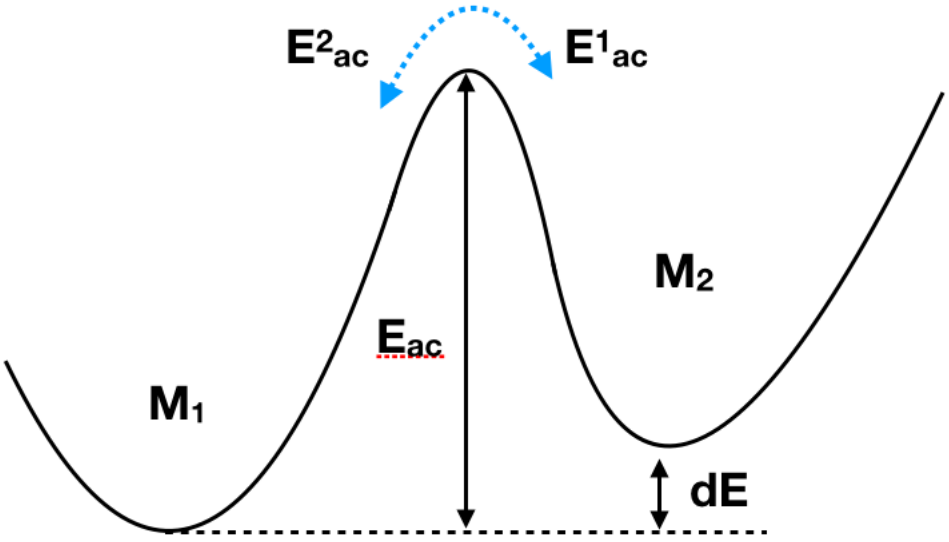

Fig. 1: Asymetric barrier between two locals minimum.

On one line composed of atom "A" and vacancies "V", we can evaluate the value of dE as function of dandling bond and bond create after the vacancy diffusion. Here are the two configurations:

$$\begin{array}{l} ... - A - V - A - V - A - ... \;\; M_2 \\ ... - A - V - V - A - A - ... \;\; M_1 \end{array}$$

to compute the variation of bond between M_1 and M_2 we need to count the number of dandling bond and empty bond for the vacancy "V" ($ddb(V)$ & $v(V)$ respectively) and to count the number of bond and dandling bond for atome "A" ($bd(A)$ & $ddb(A)$ respectively) and we apply the formula:

$$\Delta bd = ddb(V) + ddb(A) + 2 - v(V) - bd(A) \tag{1}$$

the "+2" mean we count a dandling bond twice between A and V.

For event from configuration M_1:

$$\begin{array}{ll} ddb(V) = 2; & bd(A) = 0 \\ v(V) = 0; & ddb(A) = 2 \end{array} \Rightarrow \Delta bd = 2$$

For event from configuration M_2:

$$\begin{array}{ll} ddb(V) = 1; & bd(A) = 1 \\ v(V) = 1; & ddb(A) = 1 \end{array} \Rightarrow \Delta bd = -2$$

Implementation step by step

We will work on the file Ex02.f90 or Ex02.c according to your preference. We can see that the routine read_event is already write to read the event parameters (init_state, final_state, f0, ebarrier and de) and the energy bond between two site's state. So we will concentrate on the routine event_rate_calc. We must know that the atom "A"

Algorithm 1 Compute the activation energies as function of the site's environment

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LOOP "i" in tot_sites:

IF state's site of "i" is not a vacancy:
next "i"

LOOP "j" on i's neighbors:
count ddb(i) & v(i)
END LOOP

IF no atom "A" neigbour:
next "i"

LOOP "j" on i's neighbors:

LOOP "k" on j's neighbors:
count bd(j) & ddb(j)
END LOOP

Compute Dbd of this event (eq.1)

Compute the rate between "i" and "j" in "event_rate"

ADD in "rate" the total rate of site "i"

END LOOP

END LOOP
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are represented by the state 1 and the vacancies by the state 0. To write the algorithm to compute the rate for all possible event in the system we will consider only the vacancies which have an atom A as neighbour. We can write in the way describes in Algorithm 1:

In analyse routine it is already implemented an algorithm to compute the average size of cluster of vacancies. Like that you can follow this properties during the kinetic.

Advice

You can process by step:

1. Write the algorithm to compute the rate of each event without take into account the environment
2. Insert the part to take into account the environment

Application

Run your code for a 2 dimensions systems 128x128 with priodic boundary condition in x and y and 2 node state possible. Use the algorithm you want BKL or Gillepsie and use "init_conf" random with 0.10 the fraction of vacancies in your system.

Optimisation

As in the first exercice, at each step the algorithm write before pass through all the site of the system and recompute the rate of event that are no change.

1. It is intersting to save the site that is change at the previous step and the neighbors site. So we save a group of site in the array that will not exceed 10 elements (from my point of view). This step can be done when the site is change, in event_applied routine using a global variable.

2. Now in event_rate_calc routine we will go through the list of site whose the environment have probably change. In the principal loop "i" on "tot_sites" replace "tot_site" by the number of site you have save previously and compute the event_rate for "is = list[i]" for instance.

3. An important remark is to re-initialize at zero the arrays "rate" and "event_rate" when the state of the site become "1"

The temperature effect

If you run this system you can see that the vacancies prefer to form a cluster. You can see the effect of temperature on this trend. In analyse routine is implemented an algorithm which count the size of the cluster in system and make an average. With it you can follow the average size of the cluster during the simulation. We want see the temperature effect on this average size. You know that the rate is proportional of ratio $\frac{E_{ac}}{k_B T}$, so in "input_KMC.dat" file you can initialize directly the value of $k_B T$ with the keyword "kT".

Run the simulation for differents values of $k_B T$ proportional to J the value of energy bond between atom "A": $k_B T = \{-J, -{}^{3J}/_{2}, -2J, -3J\}$. In the same graph, plot the cluster size average as function of time of all simulation. Comment the graph.