FAU

Friedrich-Alexander-Universität
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WW8: Materials Simulation

Practical: Kinetic Monte Carlo Simulation

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Contents

1 Introduction

The Monte Carlo method broadly refers to a large toolset of modelling methods utilizing the generation random numbers to solve problems. The underlying algorithm is the Metropolis algorithm. As opposed to Molecular Dynamics Monte Carlo methods do not follow the simulated particles trajectories over, but randomly perturbed the system to asses the the resulting systems properties in comparison to the preceding system. The *Kinetic Monte Carlo* (KMC) method incorporates kinetic features to the simulation. Each transition from state to state is seen is a diffusive jump and can happen at timescales larger than in Molecular Dynamics (which is limited by the time-scale of atomic vibrations) [1].

1.1 General Algorithm of the rejection free KMC Method

We start with a system of possible states i and possible transitions $i \to j$. The transition rate is ν_{ij}. The following algorithm is reproduced from the problem statement [2].

1. start with state i at time t

2. evaluate total jump rate Γ

$$\Gamma = \sum_j \nu_{ij} \tag{1}$$

3. evaluate probability of jump by comparing ν_{ij} to the total jump rate (eq. 2a) and calculate the cumulative probability 2b

$$p_j = \frac{\nu_{ij}}{\Gamma} \tag{2a}$$

$$P_j = \sum_{j'<j} p_{ij'} \tag{2b}$$

4. generate a random number $R_1 \in [0,1)$

5. chose state which satisfies $P_{ij} = \min P_{il}, P_{il} > R_1$ (where P_{il} is a list ordered in descending order, to make sure that high probability steps are more likely to be executed)

6. generate random number $R_2 \in [0,1)$ and calculate jump time t_{ij} as

$$t_{ij} = -\frac{\ln(R_2)}{\Gamma} \tag{3}$$

7. update system configuration: $i \rightarrow j$ and update time $t = t + t_i j$

8. restart loop

2 Diffusion Problems Solved with KMC

2.1 Diffusion in a Cu thin film with time dependent diffusion rate

In this task we consider a sandwich structure of a Cu film and a Cu-10% Al film, both of thickness 100 nm. As Cu is an fcc-metal it is possible to simplify the set-up to a 2D simple cubic lattice. The diffusion coefficient is given as:

$$D = 1.49 \cdot 10^{-7} \exp\left(-\frac{136.1\text{kJ}}{\text{RT}}\right) \frac{\text{m}^2}{\text{s}} \tag{4}$$

In 3D-the jump rate for e.g. Carbon at octahedral interstitial sites in α-iron is given as [3]:

$$\nu_{ij} = \frac{6D}{b^2} \tag{5}$$

so for a 2D-simple cubic with 4 possible moving directions it should be given as:

$$\nu_{ij} = \frac{6D}{b^2} \tag{6}$$

The jump rate ν_{ij} can be derived from D as follows:

$$\nu_{ij} = \frac{4D}{b^2} \tag{7}$$

with $b = 2.54$Å. As we are considering only one kind of diffusion process ν_{ij} is the same for all jumps so eq. 1 simplifies to:

$$\Gamma = n\nu_{ij} \tag{8}$$

and the probability from eq. 2a simplifies as stated below:

$$p_{ij} = \frac{\nu_{ij}}{\Gamma} = \frac{1}{n} \tag{9}$$

where n is the number of jumps.

References

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2. Zaiser, M. *Kinetic Monte Carlo Simulation - Problem Statement*

3. Gottstein, G. in *Physical Foundations of Materials Science* (ed Gottstein, G.) 155–196 (Springer, Berlin, Heidelberg, 2004). ISBN: 978-3-662-09291-0. `https://doi.org/10.1007/978-3-662-09291-0_6` (2024).