Data article

Data sets of migration barriers for atomistic Kinetic Monte Carlo simulations of Fe self-diffusion

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\textbf{Abstract}
Atomistic rigid lattice Kinetic Monte Carlo (KMC) is an efficient method for simulating nano-objects and surfaces at timescales much longer than those accessible by molecular dynamics. A laborious and non-trivial part of constructing any KMC model is, however, to calculate all migration barriers that are needed to give the probabilities for any atom jump event to occur in the simulations. We calculated three data sets of migration barriers for Fe self-diffusion: barriers of first nearest neighbour jumps, second nearest neighbours hop-on jumps on the Fe \{100\} surface and a set of barriers of the diagonal exchange processes for various cases of the local atomic environments within the 2nn coordination shell.

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### Specifications table

| Subject area            | Physics                                                                 |
|-------------------------|------------------------------------------------------------------------|
| More specific subject area | KMC simulations of surface diffusion                                  |
| Type of data            | Table                                                                  |
| How data was acquired   | Nudged Elastic band calculations with semi-empirical potentials        |
| Data format             | raw                                                                    |
| Data source location    | Helsinki, Finland                                                     |
| Data accessibility      | data is with this article                                             |

### Value of the data

- *Fe Set 1, Fe Set 2NN and Fe Set Exchange* tables of migration energy barriers can be used for atomistic rigid lattice Kinetic Monte Carlo simulations of self-diffusion on arbitrarily rough surfaces via first and second nearest neighbour jumps and diagonal exchange processes.
- Bulk diffusion is also possible to simulate with these data sets in KMC.

1. Data

*Fe Set 1* and *Fe Set 2NN* tables accompanying this article contain 5 columns named *a*, *b*, *c*, *d*, *Em*, where *a* and *b* are the numbers of first nearest neighbours (1nn) and second nearest neighbours (2nn) of the initial configuration of the jumping atom, respectively; *c* and *d* - the corresponding numbers for the final vacant lattice site (*c* in *Fe Set 1* and *d* in *Fe Set 2NN* include the jumping atom itself in its initial position); *Em* is the energy barrier in eV, which the jumping atom needs to overcome in order to make a transition from its initial configuration to the final vacant lattice site. The description where the barrier is described by the number of 1nn and 2nn atoms will henceforth be called the 4D parameterization. *Fe Set 1* includes the barriers for 1nn jumps; *Fe Set 2NN* – 2nn hop-on jumps on the Fe (100) surface.

*Fe Set Exchange* includes the barriers of the diagonal exchange processes on Fe (100) surfaces for all possible combinations (excluding the symmetric ones) of 2nn atoms of the initial adatom and the final position of the dislodged surface atom. *Fe Set Exchange* has the following format:

\[ s_0 \ s_1 \ s_2 \ s_3 \ s_4 \ s_5 \ Em \]

where \( s_0, \ldots s_5 \) are the occupation states (1 = occupied, 0 = vacant) of the six 2nn adatoms' sites around the initial adatom and the final position of the dislodged surface atom, *Em* is the corresponding barrier value in eV. All sets are described and analysed in detail in [1].

2. Computational methods

*Fe Set 1* and *Fe Set 2NN* were constructed within 4D parameterization scheme of the KMC code Kimocs [2]. In the 4D description of the atomic jumps, only the numbers of 1nn and 2nn of the initial and final sites of the transition are taken into account, but not the precise arrangement of these neighbours (see Fig. 1 for an example of a 2nn jump). Thus, a single value of the energy barrier is assigned to the whole set of various permutations corresponding to the same \((a, b, c, d)\) 4D vector. Such an approach significantly reduces the set of necessary barriers within the 2nn coordination shell from \( \sim 10^5 \) down to \( \sim 2000 \) for 1nn jumps in body-centred cubic (BCC) lattice structures.

*Fe Set Exchange* consists of the barriers of the diagonal exchange processes on Fe (100) surface for all possible combinations of 2nn within the same monolayer as the initial adatom and the final
position of the dislodged atom. In Fig. 2, the initial adatom on top of the Fe {100} surface is shown in green. It dislodges the yellow surface atom and takes its place. The yellow atom is forced to become an adatom and takes the diagonal hollow vacant site (between the adatoms 3, 4, 5 and 6). Numbered adatoms are 2nn adatoms of the initial green adatom and a final hollow site position of the yellow atom.

All the barriers in all three sets were calculated using the Nudged Elastic Band (NEB) method [3,4] with the EAM interatomic potential, developed by Mendelev et al. [5]. The initial and final configurations of every process were constructed in a rigid lattice, either on a surface or in bulk (see [1] for details). During the initial relaxation stage, the initial and final configurations of the processes were relaxed with the conjugate gradient method. The straight line from the relaxed initial position to the relaxed final one was chosen as the initial guess of the minimum energy path (MEP) for 1nn and 2nn jumps. The interpolation path for diagonal exchange processes was chosen to go through the state, in which both the adatom and the surface atom occupy the same lattice site. The minimization of the
interpolated path towards the minimum energy path (MEP) was handled by the NEB algorithm in the Molecular Dynamics code PARCAS [6–8]. We used the approach described in [9] for the calculation of the additional NEB spring force between the images. A sequence of 40 images was used for every jump. The initial and final images were relaxed with the conjugate gradient method and then fixed during the NEB calculations. The energy barrier is found from the relaxed MEP as a difference in the potential energies of the configuration at the saddle point and the initial configuration.

**Fig. 3.** Table of energy barriers of adatom exchange events with various local atomic environments of the jumping adatom and the surface atoms involved in substitution. Processes are described by 6 numbers: $s_0$ $s_1$ $s_2$ $s_3$ $s_4$ $s_5$ $E_m$, where $s_0$, … $s_5$ are the occupation states (1 = occupied, 0 = vacant) of the six 2nn adatom sites around the initial adatom and the final position of the dislodged surface atom. $E_m$ is the corresponding barrier value in eV. The presented neighbours are shown in blue color.
Some processes in Fe Set 1 were identified as spontaneous during NEB (see [1,10] for details) and assigned the barriers with the following heuristic formula:

\[ E_m(a, b, c, d) = \epsilon a + \delta b + \epsilon c^{-1} + \delta d^{-1} \]  

(1)

where \( \epsilon = 10^{-3} \, \text{eV} \) and \( \delta = 10^{-4} \, \text{eV} \). This formula is designed to prioritize the jumps of atoms with the fewest neighbouring atoms. It also assumes that it is more favourable for an atom to jump into a position with a higher number of neighbours. \( \epsilon \) and \( \delta \) are chosen so that the number of 1nn atoms contributes more into the value of migration barriers than the number of 2nn atoms.

Fe Set 1 includes 1760 barriers, most of which were calculated in the bulk. Barriers for jumps on the \{110\} surfaces were calculated separately and are prioritized in this set. 214 barriers were assessed by using Eq. (1). Fe Set 2NN contains 16 \((a, b, c, d)\) barriers for the direct jumps of adatoms to a vacant 2nn site on the \{100\} surface. The permutations for each event in Fe Set 1 and Fe Set 2NN were combined and used in [11], where the attempt frequency for all events was assumed to be \( \nu_D = 6 \cdot 10^{12} \, \text{s}^{-1} \) [12].

Fe Set Exchange includes 36 barriers. Barriers of various arrangements of numbered 2nn, which are included in Fe Set Exchange, are illustrated in Fig. 3 for readers’ convenience. Blue squares mean that the numbered adatom is present, white squares correspond to the situations where 2nn sites are vacant. Fig. 2 correspond to the lower right corner case in the table in Fig. 3.

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Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2018.04.060.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi: http://dx.doi.org/10.1016/j.dib.2018.04.060.

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