

User's Manual for LAMOCA

A Kinetic Lattice Monte Carlo Simulator for
Study of Point Defect Mediated Dopant Diffusion in Silicon

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Chapter 1 Introduction

1.1 Introduction

Lamoca is a 3D atomistic simulator designed to investigate point defect-mediated dopant diffusion in silicon at elevated process temperatures. Some of its fundamental features include:

- It is based on a stochastic method.
- The domain it operates on is a silicon lattice (cF8) and high symmetry points (tetrahedral, hexagonal and bond-centered).
- Dopant atoms and point defects (vacancies and interstitials) are mapped onto a perfect silicon lattice domain.
- Only point defects are mobile; dopants diffuse via interaction with point defects. A point defect diffuses via reaction with its first nearest neighbors (1NNs). A vacancy moves through exchanging its position with one of its four 1NNs.
- A split interstitial moves by completing both a dissociation process that the split interstitial breaks apart in its current site and an association process that one of the two constituents jumps into one of its 1NNs, resulting in formation of a new split interstitial.
- The reaction rates of these aforementioned processes are calculated based on the change of the system energy due to the process.

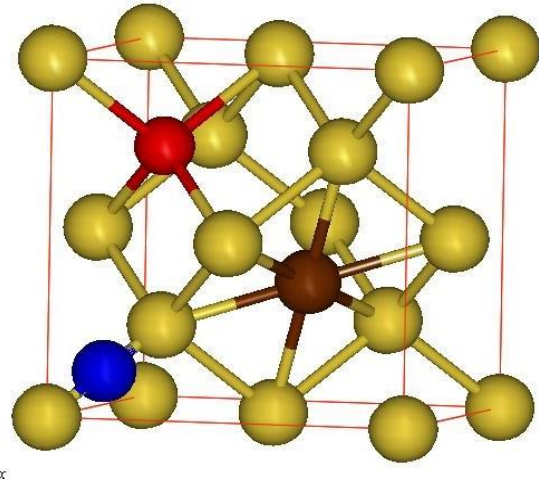
1.2 Simulation Domain

The KLMC simulation domain consists of a large number of discrete sites on which atomic species can transition from one site and/or configuration to another. The unit cell of the domain is the crystalline silicon cubic structure which consists of eight substitutional lattice sites. In addition, we augment the constituent sites to include high symmetry sites which are involved in diffusion processes as listed in Table 1. Illustrations of all these sites in one unit cell are shown in Figure 1. The simulation domain includes a three-dimensional array of such cubic cells using three-dimensional periodic boundary conditions.

Table 1. Sites in the unit cell of the simulation domain and their numbers per cubic cell. A substitutional site is simply the silicon lattice site. A tetrahedral site is at the center of a tetrahedron formed by 4 substitutional sites. A hexagonal site is at the center of a hexagonal ring formed by 6 substitutional sites. A bond-centered site is at the center of a Si-Si bond. Lattice coordinates for typical substitutional, tetrahedral, hexagonal and bond-centered sites are (0, 0, 0), (1/4, 1/4, 3/4), (5/8, 3/8, 3/8), and (1/8, 1/8, 1/8), respectively.

Sites	Numbers	Abbreviations
Substitutional (S)	8	sub
Tetrahedral (T)	8	tet
Hexagonal (H)	16	hxg
Bond-centered (B)	16	bon

Figure 1. Illustration of sites in the unit cell of the simulation domain: substitution sites (light/yellow), a tetrahedral site (dark/red, upper left), a hexagonal site (dark/brown, right) and a bond-centered site (dark/blue, lower left).



1.3 Species

In its current version, Lamoca is capable of simulating diffusion processes involving major impurities in silicon. Each defect species is characterized by three properties: constituent atom, occupying sites, and orientation. Some definitions are below:

- Simple defect: A defect that is composed of only one constituent atom, such as a substitutional phosphorus or a vacancy.¹
- Complex defect: A defect that is composed of two atoms.² It is also called an interstitialcy.
- Intrinsic defect: A defect that is composed of only silicon and vacancy, e.g. a vacancy or a silicon interstitial on a hexagonal site.
- Extrinsic defect: A defect that includes impurity atom(s), e.g. a carbon-silicon interstitialcy on a substitutional site.

The atom species included are listed Table 2. Complex defects may include two of the atom species. For example a silicon-silicon interstitialcy contains two silicon atoms.

Table 2. Atom species and symbols.

Atom Species	Symbol
phosphorus	P
carbon	C
arsenic	As
germanium	Ge
boron	B
silicon	Si
Vacancy ³	V

Depending on what type of sites these defects reside on, we can further distinguish in Table 3.

¹ Here we treat vacancy as a simple defect consisting of a “vacancy” atom.

² Now we only include complex defect on substitutional sites.

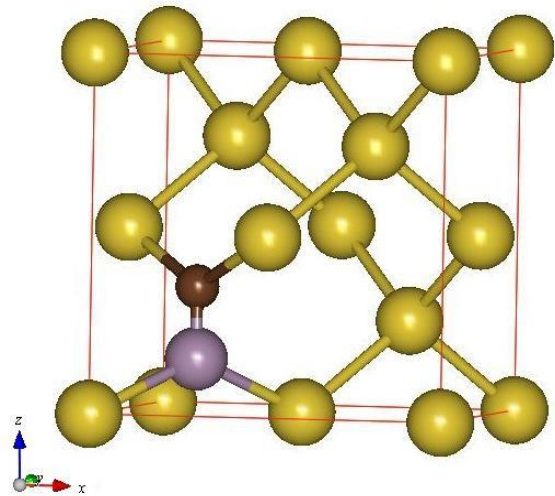
³ Vacancy is only on substitutional sites. If there is nothing on augmented sites, we call it a “blank” species.

Table 3. Naming convention of defects.

name of constituent atom species	site type abbreviation	name	e.g
X	S = sub	X	phosphorus; vacancy
X	S= hxg/tet/bon	X_S_interstitial	carbon_hxg_interstitial; phosphorus_tet_interstitial;
X,Y	S=sub	X_Y_interstitialcy	carbon_phosphorus_interstitialcy; silicon_silicon_interstitialcy germanium_silicon_interstitialcy;

Orientation only applies to complex defects. It is defined as the vector pointing from the first constituent atom to the second. Figure 2 displays a [001] oriented carbon_phosphorus_interstitialcy

Figure 2. A [001]-carbon-phosphorus interstitialcy in silicon lattice (yellow). Orientation goes from phosphorus (large, purple) to carbon (small, brown).



1.4 Major Transitions

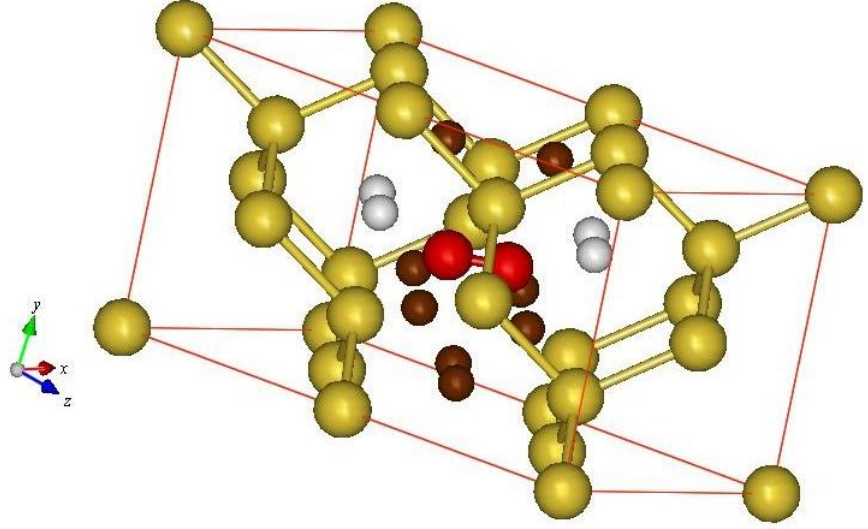
In KLMC, a transition is a process in which an atom jumps from one site and/or configuration to another. Here we only consider transitions that are associated with diffusion. There are two major categories of diffusion mechanisms for diffusion in Si, namely vacancy and interstitial mechanisms. The vacancy mechanism involves a siliconvacancy exchange process, which is simply: vacancy+silicon \Leftrightarrow silicon+vacancy. The interstitial mechanism involves the formation and dissociation of interstitials. For example the silicon self diffusion involves:

silicon_hxg_interstitial + silicon \Leftrightarrow silicon-silicon interstitialcy + blank_hxg.

We sometimes need to take into account the orientation constraint, which implies that for the most energetically favorable transition the hopping directions and the split orientations are the most closely aligned. This limits the number of possible hops. For example for a silicon-silicon interstitialcy, there are 12 neighboring hexagonal sites; however, for any specific orientation, only 4 sites are accessible, 2 for each of the atoms forming the split interstitial. Figure 3 shows the 12 hexagonal neighbors around a lattice site and the 4 accessible sites for the orientation pictured. Similarly, when a hexagonal interstitial hops to a substitutional site, the orientation of the resulting

interstitialcy has limited choices. The transitions together with orientation limits are specified in the transitions.inp file.

Figure 3. The 12 neighboring hexagonal sites (small spheres) of a [101] split interstitial (dark/red bonded pair, big spheres). The 4 light/white ones are accessible sites and the 8 dark/brown ones are not.



1.5 System Energies

The energy of the system is defined as follows:

$$E = E_f + E_b = \sum_i E_f^i + \sum_{i<j} E_b^{i,j} \quad (1)$$

where i and j run through all the defects and impurities in the system. The first term is the total formation energy of all species, which is dependent on external stress. The formation energy of a species in the presence of an external applied stress, σ , is calculated as:

$$E_f = E_{f0} - V_0(\Delta\epsilon \cdot \sigma) \quad (2)$$

where E_{f0} is the formation energy under the stress-free condition, V_0 is the atomic volume of silicon lattice, and $\Delta\epsilon$ is the induced strain of the point defects/impurities. Both stress and strain tensors are written in the contracted notation.

The second term is the binding energy, which is a measure of binding strength between a pair of defects/impurities. The binding energy is the sum of all pair energies of the system, extending from 1st nearest neighbors (1NNs) to n^{th} nearest neighbors (nNNs). In our current version we can track interactions up to 3NNs.

1.6 Transition Rates.

In KLMC, each transition is associated with three states, which are initial, transition, and final states. The rate of a transition is an Arrhenius function of the associated migration barrier E_m :

$$v = v_0 \exp\left(\frac{E_m}{kT}\right) \quad (3)$$

where v_0 is the attempt frequency, and T is the system temperature. The migration barrier can be expressed as the sum of E_{m0} , an unbiased barrier, plus the change of barrier due to other effects, such as pair binding and external stress. Table II lists the unbiased stressfree barriers of transitions included in this work, as obtained from DFT calculations. The change in migration barrier due to

other effects can be expressed as a combination of the change in state energies that satisfies detailed balance.

$$E_m = E_{m0} + \left(\Delta E_{tr} - \Delta E_{in} + \frac{\Delta E_{fi} - \Delta E_m}{kT} \right) \quad (4)$$

where ΔE is the change in state energies due to pair binding and applied stress, and the subscripts *in*, *tr* and *fi* represent initial, transition and final states respectively. Table III and Table IV are induced strain vectors used to calculate the change in state formation energies via Equation (2).

1.7 Simulation Procedure.

In Lamoca the system evolves by virtue of reactions between point defects and their 1NNs. A step in Lamoca terminology is defined as a completion of a reaction process. Reactions are carried out sequentially so simulations proceed step by step. Logically, each simulation follows the way described as below:

- 1) At start, calculate rates for all possible reactions in the system. According to rate calculations involve computing system energy before and after a reaction.
- 2) Compare all the rates and choose one reaction from the possible set. The chance that a reaction may be selected is directly proportional to the value of the rate of the reaction.
- 3) Perform the selected reaction.
- 4) Increment the system time by the inverse of the sum of all possible transitions rates:

$$\Delta t = \frac{1}{\sum_N \nu_N} \quad (5)$$

- 5) Calculate rates for new reactions and update rates for old reactions in case their rates have been affected by the previous reaction. As a result of a reaction, the system configuration is locally altered. This may effect on the energies of nearby potential reactions and for this reason, change their rates.
- 6) Repeat from step (2) to step (5) until user-defined conditions are met.

Chapter 2 Input files

2.1 parameter.inp

The "parameter.inp" input file accepts formatted user input of the following parameters:

- The size of the domain on which the simulation is executed.
- The system temperature value (for the current version temperature is constant over all regions.)
- The impurity (dopant and point defect) type and its initial concentration within the domain.
- The timing factors of the simulation (e.g. , process time).
- The output information.

Each input line within this file is either a comment line distinguished by a leading "#" sign or, a command line defining one of these aforementioned parameters. Each command line starts with a keyword followed by parameters. The following is a description of all commands.

`size x_size y_size z_size`

This command defines the dimension of the simulation domain, measured by the silicon lattice constant. All supplied size values must be integers. How big the simulation domain can be is limited by the computing resources, especially the memory of the machine. For a machine with a one-gigabyte memory capacity, these size values should not exceed 100.

`temperature value`

This command defines the system temperature type and its value in Celsius degrees.

`timing logstep totalstep totaltime`

This command can be used to control duration of the simulation and to define the periodicity on which the system information is written to the output files. The first parameter, `logstep` defines specifies a period in steps on which the system data is snapshot and saved to the output files. A step in the simulation is defined as completion of a hop/exchange event. The second parameter, `totalstep` specifies the duration of a simulation in terms of step, while the third parameter, `totaltime` does so in terms of real time (seconds).

`boundary bc_xlo bc_xhi bc_ylo bc_yhi bc_zlo bc_zhi`

This command can be used to specify the boundary conditions of the cubic system. Currently only periodic (r) and reflective (p) conditions are supported. To specify a cube with reflective boundary condition in z direction and periodic boundary condition in other directions, this line should be written as: `boundary p p p p r r`.

`attempt_frequency value`

This command specifies the attempt frequency of each hop. Currently we only support a uniform attempt frequency for all species, which can only give the right order of magnitude of the simulation time. An approximate value is 10^{-14} s^{-1} (also the default).

`output output_item`

This command specifies what will be the output each log interval. The options are: `cube` outputs `cubiclist.out`, lists all defect species by the order of their cube index `neighbor` outputs `neighborlist.out`, lists a list of all neighbors of all defect species `rate` outputs `ratelist.out`, lists the hopping rates of all possible transitions. `diffusivity` outputs `diffusivity.out`, lists the diffusivities of all the species present. `lattice` outputs defect positions. `all` outputs all the files above.

The same command may be executed multiple times with the last superseding all previous ones.

2.2 defect.inp

defect.inp specifies the number and location of species in the system. The species should exist in the database. There are two ways to initialize a defect distribution: manually or randomly.

To initialize the distribution randomly, the following format should be adopted:

```
defect=defect_species random
number=defect_number density=defect_density
region=(xmin,xmax,ymin,ymax,zmin,zmax)
orientation=<defect_orientation>
```

The first line specifies the defect species followed by the keyword “random”. The second line contains several keywords. Either number or density can be specified. If `density` is used, then the defect number is the product of the density value and the region volume rounded up to the closest integer. `region` specifies the region where the defects are initialized. Like the size command, the values here are in units of silicon lattice constant. This region should not extend out of the domain size. `orientation` is the set of orientations for the initial defects. It can be omitted if the defect has no orientation (e.g., for simple defects).

To initialize the distribution manually, the following format should be used:

```
defect=defect_species manual
Defect_number
x1 y1 z1
x2 y2 z2
...
```

The first line specifies the defect species followed by the keyword “manual”. The second line specifies the number of defects. The list of defect coordinates starts from line three. The number of lines specifying coordinates should be the same as the number in the second line.

2.3 transition.inp

transition.inp specifies all the allowed reactions in the system. The species should exist in the database. The reaction of the species is specified as follows

```
REACTION species1 + species2 = species3 + species4
ORIENTATION index(1-4)=index cos_angle=cos_value
FORMATION_ENERGY initial=value transitional=value final=value
```

The first line specifies the reactants and products of the species. If the species has an orientation, the orientation should follow after the species name with a whitespace, like (e.g., `carbon_silicon_interstitialcy <100>`).

The second line specifies any orientation constraint on the reaction. The constraint is specified as the cosine value of the angle between the allowed hop vector and the species orientation. The first keyword `index(1-4)` specifies which species in the above reaction are under the constraint.

The second keyword `cos_angle` specifies the cosine value for the allowed transitions. If no orientation constraint is present, this line can be omitted.

The third line specifies the energy values of the different states of the reaction, in units of meV. These values are stress-free values. Energy barrier is calculated with these values.

Here is an example of a typical reaction of impurity-interstitial dissociation:

```
# silicon-self-interstitialcy dissociation
REACTION silicon_silicon_interstitialcy <110> + hxg_blank
        = silicon + silicon_hxg_interstitial
ORIENTATION index(1-4)=1 cos_angle=0.852802865
FORMATION_ENERGY initial=3700 transitional=4050 final=3800
```

It specifies forward and reverse barriers of 0.35eV and 0.25eV respectively.

2. 4 energy.inp

energy.inp specifies any 1NN binding among defect species. The format is:

```
BINDING species1 species2 value
```

The energy value is again in meV. For example a 1NN binding between substitutional arsenic and vacancy is specified as:

```
BINDING arsenic vacancy 1250
```

Chapter 3 Output Files

The output files are written at each log step, which is specified in the parameter.inp file.

3.1 lattice.out

This file contains information of positions of all defects in xyz format.

3.2 defect_array.out

This file contains information of each defect, such as species, orientation, location etc.

3.3 cube_array.out

This file contains information of each defect, ordered by the index of the cube (silicon cubic unit cell) that they reside in.

3.4 neighbor_list.out

This file contains information of all the neighbors of defects.

3.5 rate_list.out

This file contains information of the rates of all possible hops associated with each mobile defect.

3.6 hop_reaction.out

This file contains information of the hop reaction that has been selected for each time step.

3.7 log.out

This file contains information of the simulation such as parameters and initializing conditions.

3.8 diffusivity.out

This file contains information of the diffusivity of each defect species for each time step.

Chapter 4 Examples

4.1 A simple Vacancy-Mediated Arsenic Diffusion Experiment

In this example a system of multiple arsenic atoms and a single vacancy is simulated. The mean squared distance of arsenic is measured as a function of pair energy strength between arsenic and vacancy pair. The parameters are:

- The domain size is 10 x 10 x 10.
- The system temperature is constant type of 1000 °C.
- Periodic boundary condition on all surfaces.
- There are 10 arsenic atoms and a single vacancy in the system.
- The simulation runs 100000 steps and the log period is also 10000.

The "parameter.inp" file should look like:

```
#Example: vacancy mediated arsenic diffusion
size 10 10 10

# temperature of 1000C
temperature 1000

# timing, to ensure that the system stops at 1000000 steps,
# set the second parameter to a large value.
timing 10000 100000 1e17

# output atom positions and diffusivity only
dump lattice diffusivity

# periodic boundary conditions
boundary p p p p p p

attempt_frequency 1e-14
```

The "defect.inp" file should look like:

```
defect=arsenic random number=10
region=(0,10,0,10,0,10)
defect=vacancy random
number=1 region=(0,10,0,10,0,10)
```

The "energy.inp" file looks like:

```
#1nn binding between As and V
BINDING Arsenic Vacancy 1430
```

The "transition.inp" file should look like:

```
# vacancy migration (formation 3.48eV, barrier 0.35eV)
REACTION vacancy + silicon = silicon + vacancy
FORMATION_ENERGY initial=3480 transitional=3830
final=3480

# vacancy arsenic exchange
REACTION vacancy + arsenic = arsenic + vacancy
FORMATION_ENERGY initial=3480 transitional=4120
final=3480
```

The results are in diffusivity.out and lattice.out for further processing.