Tutorial: Phonon dispersion

From GPUMD
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Introduction

- In this example, we use harmonic lattice dynamics to calculate the phonon dispersion of diamond silicon.
- All the input and output files can be found here (https://github.com/brucefan1983/GPUMD/tree/master/examples/phonon/phonon_dispersion).

Preparing the inputs

The xyz.in file

The structure as specified in the xyz.in file is diamond silicon at zero temperature and zero pressure.

The basis.in file

- The basis.in file reads:

```
2
0 28
4 28
0
0
0
0
1
1
1
1
...
```

- Here the primitive cell is chosen as the unit cell. There are only two basis atoms in the unit cell, as indicated by the number 2 in the first line.
- The next two lines list the indices (0 and 4) and masses (both are 28 amu) for the two basis atoms.
- The next lines map all the atoms (including the basis atoms) in the super cell to the basis atoms: atoms equivalent to atom 0 have a label 0, and atoms equivalent to atom 1 have a label 1.

The kpoints.in file

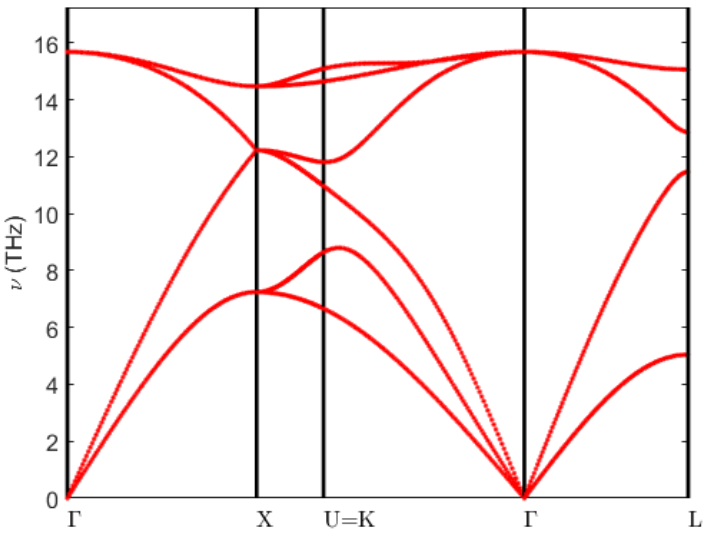
- The k vectors are defined in the reciprocal space with respect to the unit cell chosen in the basis file.
- We use the $\Gamma - X - (U = K) - \Gamma - L$ path, with 400 k points in total.

The `phonon.in` file

```
potential       potentials/tersoff/Si_Fan_2019.txt 0
cutoff          5.0 # in units of A
delta           0.005 # displacement in units of A
```

- The first line with the potential keyword tells that the potential to be used is specified in the file Si_Fan_2019.txt (https://github.com/brucefan1983/GPUMD/blob/master/potentials/tersoff/Si_Fan_2019.txt).
- The second line with the cutoff keyword tells that the force constants will be calculated with a cutoff of 5.0 A. Here, the point is that first and second nearest neighbors need to be included.
- The third line with the delta keyword tells that a displacement of 0.005 A will be used in the finite-displacement method.

Results and discussion



Phonon dispersion of silicon crystal described by the mini-Tersoff potential.

- The above figure shows the phonon dispersion of silicon crystal described by the mini-Tersoff potential [Fan 2020].

References

[Fan 2020] Zheyong Fan, Yanzhou Wang, Xiaokun Gu, Ping Qian, Yanjing Su, and Tapio Ala-Nissila, A minimal Tersoff potential for diamond silicon with improved descriptions of elastic and phonon transport properties (https://doi.org/10.1088/1361-648X/ab5c5f), J. Phys.: Condens. Matter **32** 135901 (2020).

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