Virtual Characterization Lab Toolkit

Requirements

1. You need Python 3.6 or later.

Recommended: Python 3.9 – 3.12 (well supported by NumPy/Matplotlib/SciPy).

2. Install the required libraries using pip:

pip install numpy matplotlib scipy ase

3. The workflow also requires three external programs:

LAMMPS https://www.lammps.org/download.html # For running LAMMPS
Visit https://visit-dav.github.io/visit-website/releases-as-tables/ # For visualizing SAED pattern

These must be installed and accessible in your system PATH so the scripts can call them.

4. Fonts:

The scripts use Arial. If not available, Matplotlib falls back automatically.

On Windows, Arial is pre-installed.

On Linux/WSL, you can add it with:

sudo apt install ttf-mscorefonts-installer

Implementation

Typical Usage:

python VCL-toolkit.py

Then you enter to the toolkit's interactive environment.

Preprocessing

For adding charge or spin for reactive molecular dynamics (MD) or spin-lattice dynamics (SLD) calculations, it is suggested to first making a structure file in the classical MD format. After this conversion, you can add charge or spin to the new file. If your initial structure file already has charge or spin, it will be asked to be automatically transferred to the converted LAMMPS file or set to zeros, so you will not need to perform any further conversion to add charge or spin in case you want to keep your initial charge or spin configuration. Since the current version of LAMMPS supports either charge or spin but not both simultaneously, if your file initially has charge or spin and you aim to add spin or charge, the charge/spin will be eliminated and then spin or charge will be assigned. The default assigned charge and spin values are zero for your convenience, you can add charge and spin to the atoms within the LAMMPS script itself using the `set` command. Since the initial structure is often a primitive cell, one typically prefers to enlarge it to create a supercell for Molecular Dynamics (MD) or Spin-Lattice Dynamics (SLD) simulations. Therefore, a replication option is integrated into the preprocessing step, which replicates your cell by integer numbers along the X, Y, and Z directions while keeping the stoichiometry.

LAMMPS scripts

Several LAMMPS scripts are available for spin-lattice dynamics, ReaxFF, and other simulations. These can be modified and run using the VCL toolkit based on your study's purposes.

⚠ Note: This repository of the lammps input files is intended primarily as a collection of examples. For accurate materials simulations, users should refine and adjust the parameters (e.g., magnetic and mechanical interactions) to suit their specific systems.

SAED and XRD patterns cannot be calculated for triclinic cells. To analyze a triclinic cell, you should first finalize your calculation, then convert the desired/last snapshot of the system (which is stored as a .cfg file) to the LAMMPS format using the VCL toolkit. You can then use the auxiliary LAMMPS script named in.ax to obtain the XRD and SAED patterns.

For spin-lattice dynamics, you need to adjust the system size and the number of cores used in the calculation. If your system size is too small or you use too many cores, you will receive the following error.

```
ERROR: Illegal sectoring operation (src/SPIN/fix_nve_spin.cpp:601)
```

To avoid this error, you should either reduce the number of cores or increase your system size. It is recommended to increase the system size. For more information, please see the main article.

```
article{tranchida2018massively,
title={Massively Parallel Symplectic Algorithm for Coupled Magnetic Spin Dynamics and Molecular Dynamics},
author={Tranchida, J and Plimpton, S J and Thibaudeau, P and Thompson, A P},
```

```
journal={Journal of Computational Physics},
volume={372},
pages={406--425},
year={2018},
publisher={Elsevier}
doi={10.1016/j.jcp.2018.06.042}
}
```

Postprocessing

Selected area electron diffraction (SAED)

To have a 3D analysis of your system, you should set the zone axis of the incident radiation (the zone value) to zero, i.e., `'Zone 0 0 0'`. This is specifically useful for analyzing defects. You can then use different slices along various orientations to fully analyze your desired region by changing the parameters below in VCL toolkit, which are set to provide a view along the X direction in the post-processing section for SAED pattern visualization.

spherical slice origin [39.84063, 0, 0]:
view normal vector (e.g., '-1, 0, 0') [-1, 0, 0]:
view up vector (e.g., '0, 1, 0') [0, 1, 0]:

for more information see ‘Slice operator’ in:

https://visit-sphinx-github-user-manual.readthedocs.io/en/v3.2.2/gui_manual/Operators/OperatorTypes/Slice_operator.html

However, setting Zone values to zero may require a huge amount of memory for calculations and can lead to a very large `.vtk` output file. The visualization of these large `.vtk` files also requires parallel processing and significant memory.

To avoid this, you can:

- Set the **Zone** value based only on your desired view.
- Use the `compute saed` and `saed/vtk` commands multiple times in a simulation along different directions.
- Specify only a small region for SAED analysis.

Vibrational density of states (VDOS)

There are two options for calculating Vibrational Density of States (VDOS):

Full Mode: Computes the VDOS for all atoms by analyzing their velocities in all Cartesian directions (3D).

Bond Mode: Focuses on a single bond by calculating the VDOS for the bond length fluctuations, which provides bond-specific vibrational data. If you choose Bond mode, you must provide two integers (line numbers from the .xyz file) as the IDs of your desired atoms.

Additionally, several windowing functions for the Fourier Transformation are available, including Gaussian, Blackman-Harris, Hamming, and Hann.