

Winmostar tutorial
LAMMPS
Melting point
V7.025

X-Ability Co.,. Ltd.
question@winmostar.com

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Note

- The simulation steps required are dependent on molecular species and initial density.
- The method for interaction calculations and/or the force field also affect simulation results.
- Variance in system size (number of solid phase repeats), initial temperature, and contact surface will affect results.
- For the purpose of this tutorial, the number of steps used in calculations has been limited.

Configuration

- Set up LAMMPS and Cygwin in advance.
- Set up LAMMPS by following LAMMPS Installation Guide located at https://winmostar.com/en/manual_en.html

2. Installation Guides for Solvers

For Windows

[Cygwin_wm Installation Guide](#) ※Gromacs/Amber Window Build Package(Cygwin)

(For Experts)Gromacs/Amber Build with Cygwin ※we recommend you to use the precompiled package

[GAMESS Installation Guide](#)

[NWChem Installation Guide](#) ※Window Build Package

(For Experts)NWChem Build with MinGW ※we recommend you to use the precompiled package.

[LAMMPS Installation Guide](#)

Installation guide for LAMMPS on Windows Feb. 6, 2017

1. Getting LAMMPS

① Access to <http://rpm.lammps.org/windows.html>

Visit [\[32-bit Windows download area\]](#) or [\[64-bit Windows download area\]](#).

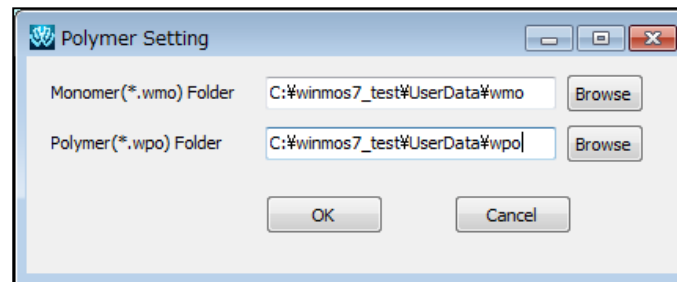
LAMMPS-ICMS Windows Installer Repository

This repository is hosting pre-compiled Windows installers of the LAMMPS molecular dynamics simulation software package. The binaries are built semi-automatically with MinGW/Linx to Windows cross compilers using up-to-date snapshots of the LAMMPS-ICMS repository hosted at the [Institute for Computational Molecular Science](#) at Temple University. The LAMMPS binaries contain all optional packages included in the source distribution except GPU (because it is not CPU compatible). OPEN_CUDA (CUDA does not support cross compilation), KOKOS and OPENMPI2 (do not support cross-compilation with GCC), USE_BUNDLED (requires external binary libraries) (requires to bundle a full Python runtime), USE_ZIPMAP (only useful when linking to a old software), USE_OPENCL (requires external library, GPU accelerated for the USE_OPENCL package which is included). The serial executable additionally does not contain the USE_MPI and USE_MPI2 packages, since those require MPIV2 functions, which are not available without linking to a real MPI library.

Some Notes on GPU Support

These Windows binaries include (experimentally on Windows) GPU acceleration via the GPU package. This is achieved through compiling the GPU package in OpenCL mode and linking to an OpenCL (v1.2) compatible GPU loader. This means the executables do not contain any vendor provided code and should be compatible with GPUs from both AMD and NVIDIA. The GPU package has been compiled for mixed precision computation and is currently somewhat tuned for Nvidia (Fermi generation) GPUs. It does not yet work with OpenCL drivers for GPUs like those included in the Intel and AMD OpenCL ICPU.

- Configuration of polymer tool Click MD | Polymer | Setting.
- Set folders for monomer files (extension .wmo) and polymer files (extension .wpo) as need.



I. Build solid phase

In this tutorial, we will calculate the melting point of silicone.

1. Click **Solid | Crystal Builder**.
2. Click **File | Open**.
3. Open **si.cif** in the sample directory. (default: C:\winmos7\samples\si.cif)

Crystal system : Cubic
 Space group : Fd-3m (227)
 Lattice constants : a=5.4309 Å
 Asymmetric unit : Si (0.0 0.0 0.0)

The screenshot shows the Crystal Builder software interface. The main window displays a 3D model of a silicon crystal structure (diamond cubic) with atoms represented by spheres. The interface includes a menu bar (File, Edit, View, Tool), a toolbar with buttons for 'a', 'b', 'c', 'a*', 'b*', and 'c*', and a status bar showing lattice constants and translation vectors.

Lattice constant 5.431 5.431 5.431 90.000 90.000 90.000
TV 5.431 0.000 0.000
 0.000 5.431 0.000
 0.000 0.000 5.431

Asymmetric Unit

Atom	X	Y	Z
Si	0.000000	0.000000	0.000000
Si	0.000000	0.500000	0.500000
Si	0.500000	0.500000	0.000000
Si	0.500000	0.000000	0.500000
Si	0.750000	0.250000	0.750000
Si	0.250000	0.250000	0.250000
Si	0.250000	0.750000	0.750000
Si	0.750000	0.750000	0.250000

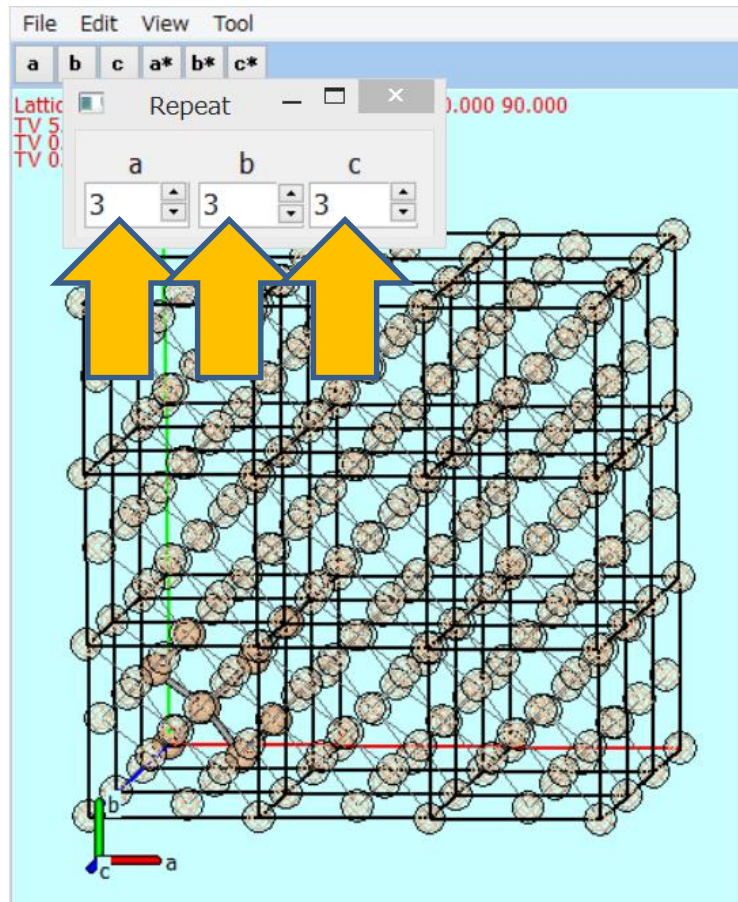
Lattice Constants
5.431 5.431 5.431 90.000 90.000 90.000

Translation Vector
5.431 0.000 0.000
0.000 5.431 0.000
0.000 0.000 5.431

Number of Atoms (displayed)
18

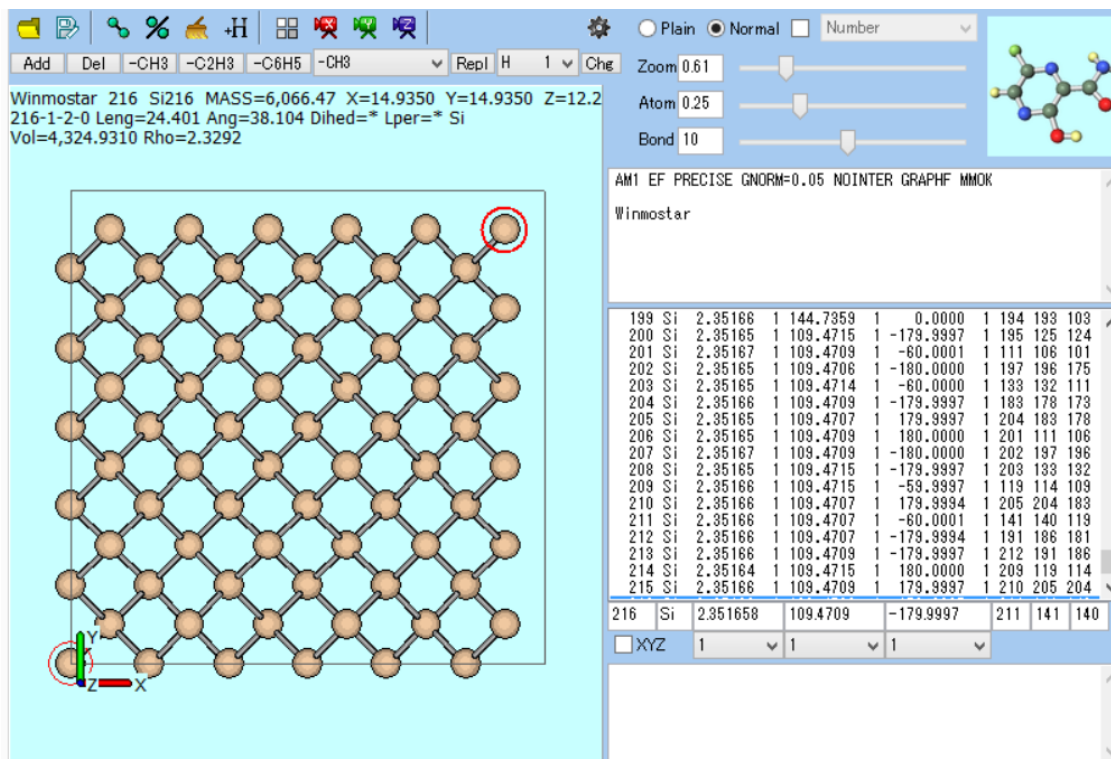
I. Build solid phase

1. Click **Edit | Repeat**.
2. Make **3 x 3 x 3** supercell.
3. Click **File | Save**.
4. Save as **si333.cif**.



I. Equilibration of solid phase

1. In **Crystal Builder**, Click **File | Exit**.
2. In **Main Window**, Click **File | Open**.
3. Open **si333.cif**.



II. Equilibration of solid phase

1. Click **MD | LAMMPS | Keywords Setup**.
2. Click **Reset**.
3. Set the following conditions.
 - Units** : metal
 - Pair Style** : tersoff
 - Potential File** : SiC_1989,tersoff
 - Ensemble** : npt
 - Time Step** : 0.0001
 - Temperature** : 2300
4. Click **OK**.

The screenshot shows the 'LAMMPS Setup' dialog box with the 'Basic' tab selected. The parameters are configured as follows:

- Extending Simulation
- Time Step [ps]: 0.0001
- Generate Velocity
- Units: metal
- # of Time Steps: 5000
- Pressure Control: iso
- Atom Style: atomic
- Ensemble: npt
- Pair Style: tersoff
- Temperature [K]: 2300
- Potential File: SiC_1989.tersoff
- Pressure [bar]: 1.013, 1.013, 1.013

The 'Keywords' section contains the following LAMMPS input script:

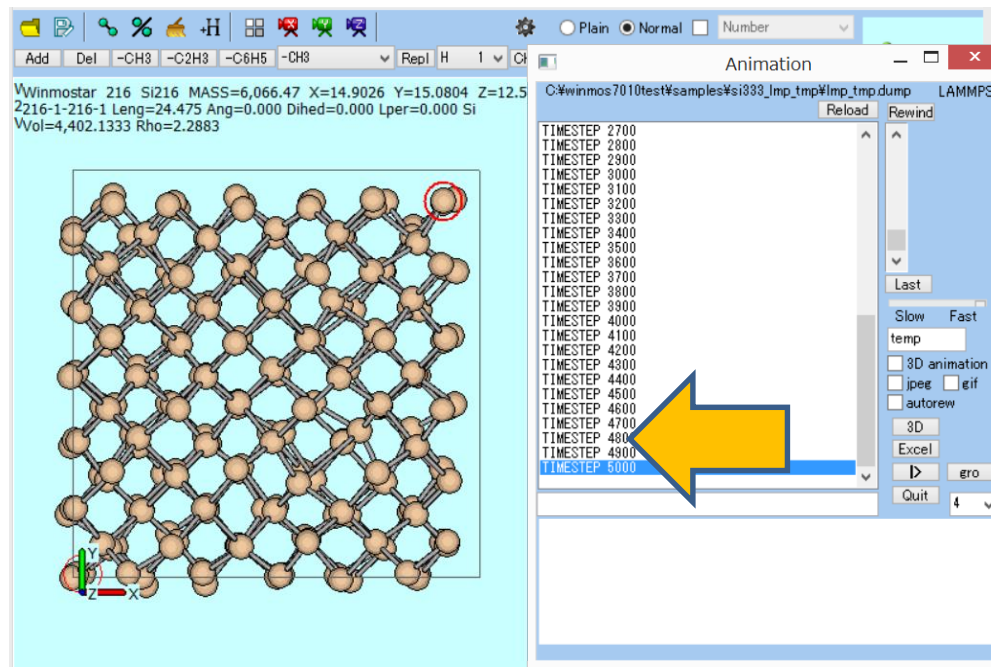
```

units metal
atom_style atomic
boundary p p p
box tilt large
read_data %DATAFILE%
pair_style tersoff
pair_coeff * * SiC_1989.tersoff %ATOMTYPES%
neigh_modify delay 0
dump 1 all custom 100 %DUMPFILE% id type xs ys zs ix iy iz
dump 2 all xtc 100 %XTCFILE%
velocity all create 2300 12345
fix 1 all npt temp 2300 2300 0.1 tchain 3 iso 1.0133 1.0133 0.1 pchain 3
fix 2 all momentum 50 linear 1 1 1
thermo_style custom step time temp pe ke etotal enthalpy press vol density lx ly lz pxx py
thermo 10
timestep 0.0001
run 5000
write_restart %RESTFILE%
  
```

Buttons at the bottom: OK, Cancel, Load Setting, Save Setting, Save as Default, Reset.

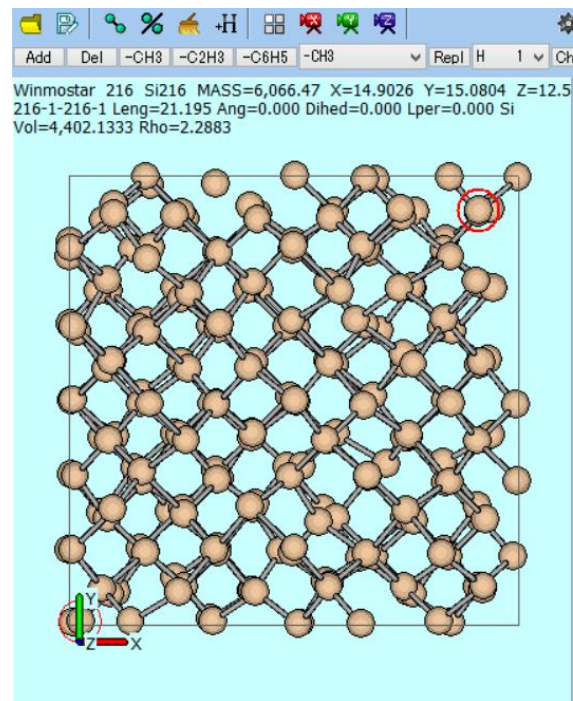
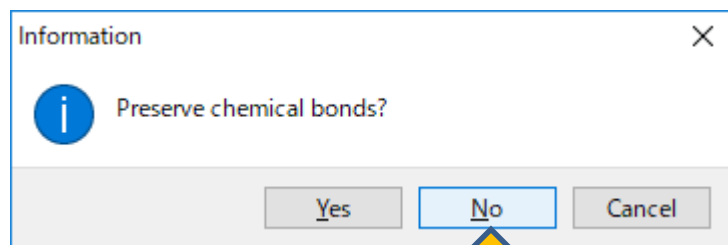
II. Equilibration of solid phase

1. Click **MD | LAMMPS | Start LAMMPS**.
2. Save as **si333.data**, then LAMMPS calculation will start.
3. After the calculation, click **MD | LAMMPS | Import Trajectory**.
4. Open the **data** file and the **dump** file selected by default.
5. Display the final step in the **Animation** window.
6. Close **Animation** window.



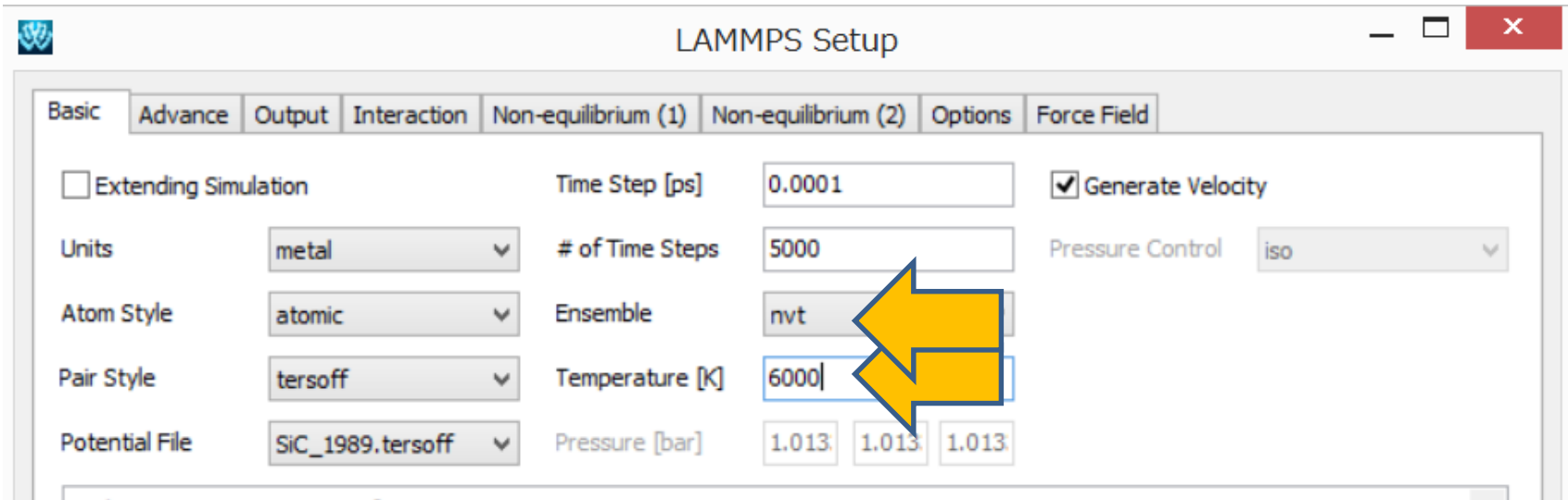
II. Equilibration of solid phase

1. Click **Edit | Pack into PBC Cell**.
2. Click **No** on the dialog.
3. Click **View | Pack into PBC Cell | Atom**.
4. Click **File | Save as**.
5. Save as **si_solid.cif**.



III. Equilibration of liquid phase

1. Click **MD | LAMMPS | Keywords Setup**.
2. Set **Ensemble** to **nvt**, **Temperature** to **6000**.
3. Click **OK**.
4. Click **MD | LAMMPS | Start LAMMPS**.
5. Save as **si_liquid.data**.



LAMMPS Setup

Basic | Advance | Output | Interaction | Non-equilibrium (1) | Non-equilibrium (2) | Options | Force Field

Extending Simulation

Units: metal

Atom Style: atomic

Pair Style: tersoff

Potential File: SiC_1989.tersoff

Time Step [ps]: 0.0001

of Time Steps: 5000

Ensemble: nvt

Temperature [K]: 6000

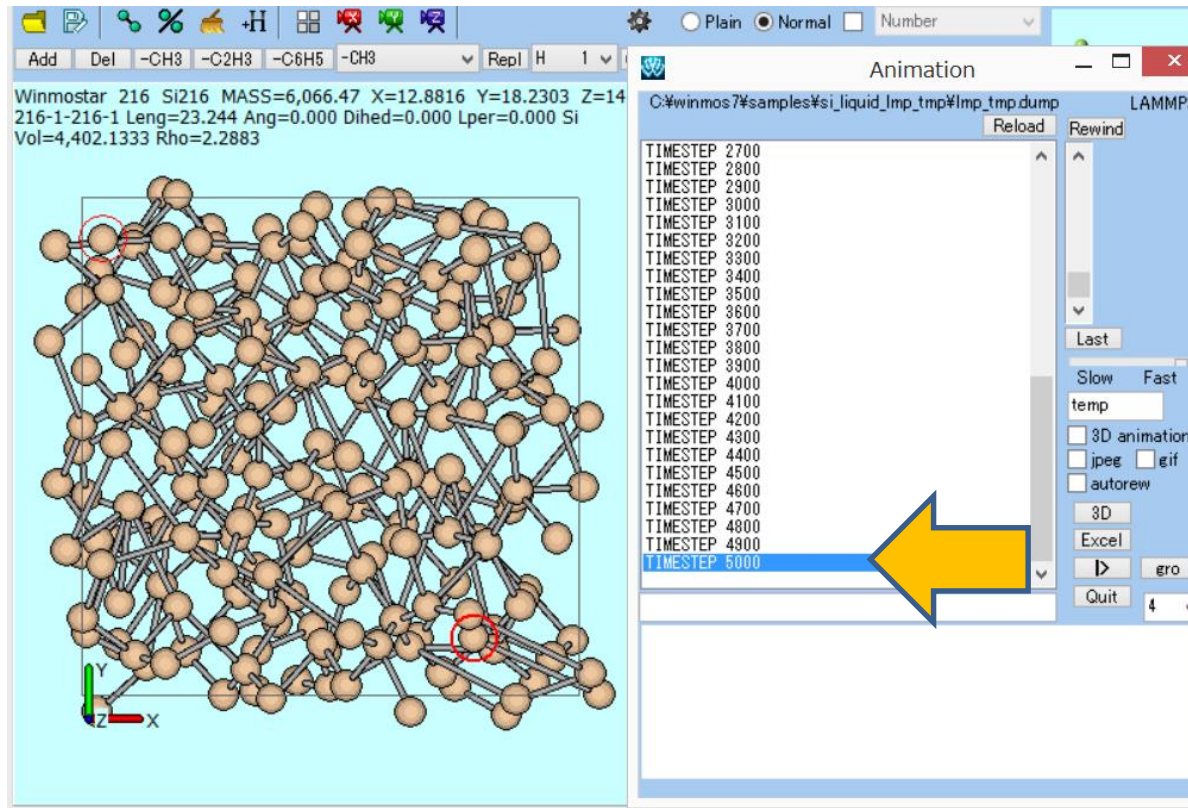
Pressure [bar]: 1.013 1.013 1.013

Generate Velocity

Pressure Control: iso

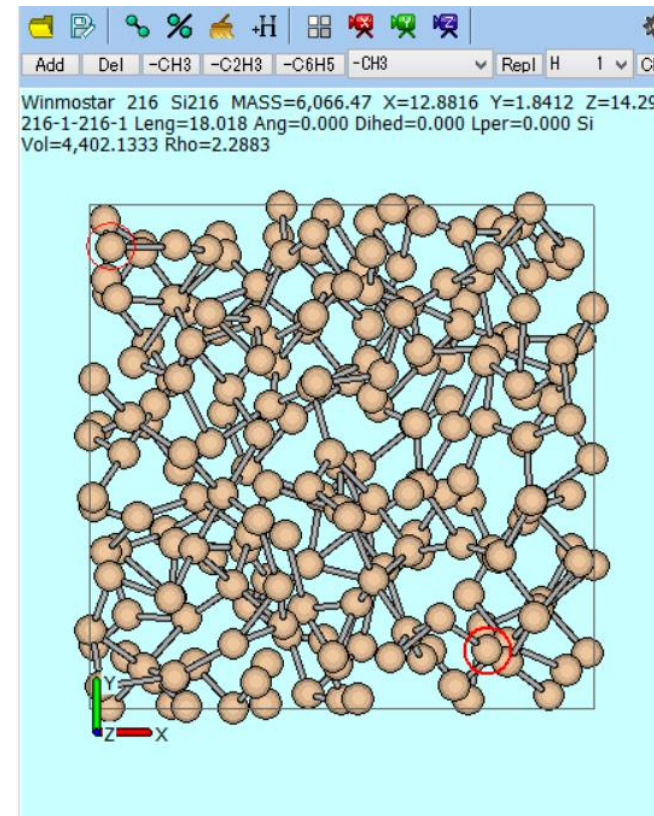
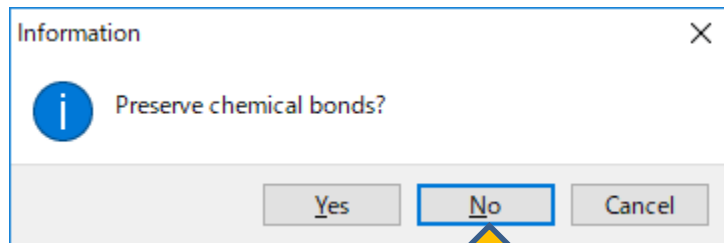
III. Equilibration of liquid phase

1. After the calculation, click **MD | LAMMPS | Import Trajectory**.
2. Open the **data** file and the **dump** file selected by default.
3. On the **Animation** window, select the final step.
4. Close **Animation** window.



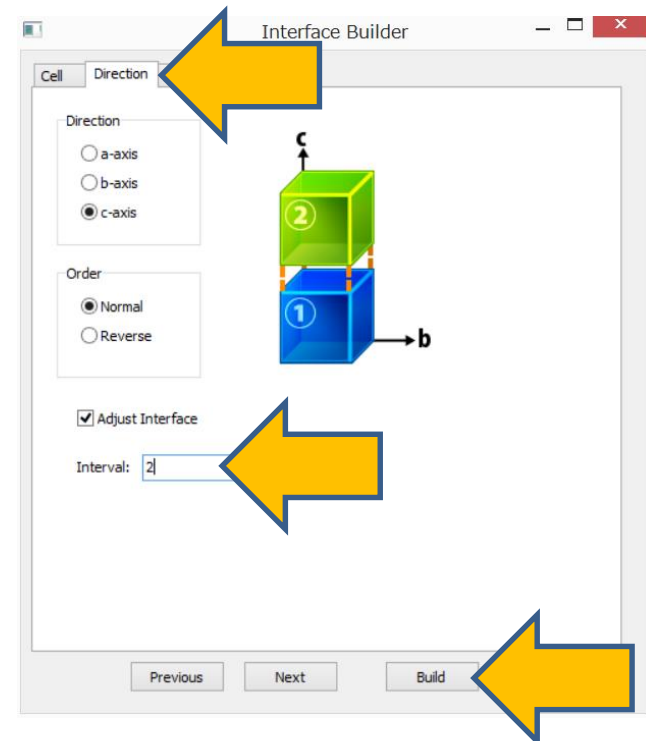
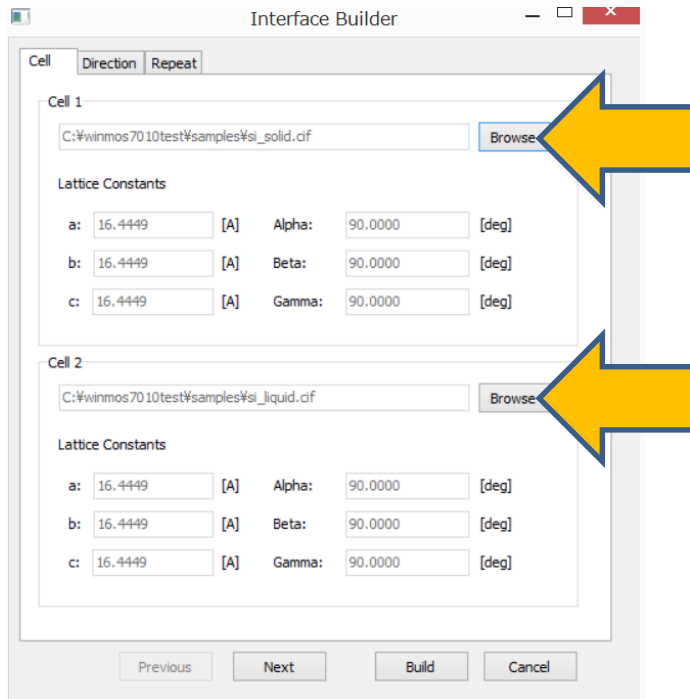
III. Equilibration of liquid phase

1. Click **Edit | Pack into PBC Cell**.
2. Click **No** in the dialog.
3. Click **File | Save as**.
4. Save as **si_liquid.cif**.



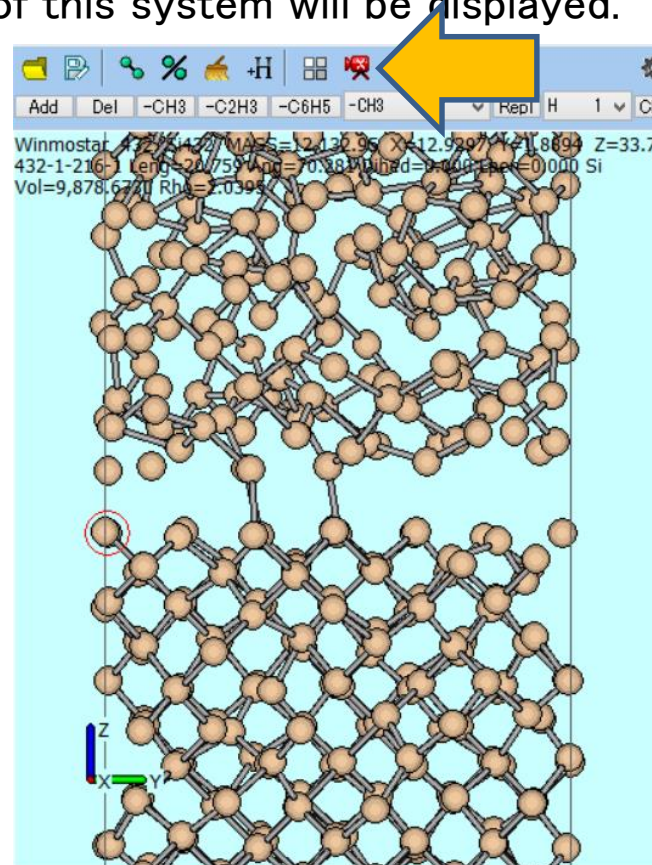
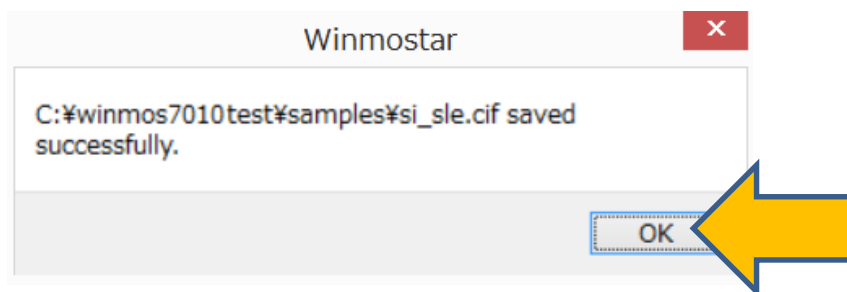
IV. Build of solid-liquid interface system

1. Click **MD | Interface Builder**.
2. Click **Browse** of **Cell 1**, then open **si_solid.cif**.
3. Click **Browse** of **Cell 2**, then open **si_liquid.cif**.
4. On **Direction** tab, set **Interval** to **2**.
5. Click **Build**.



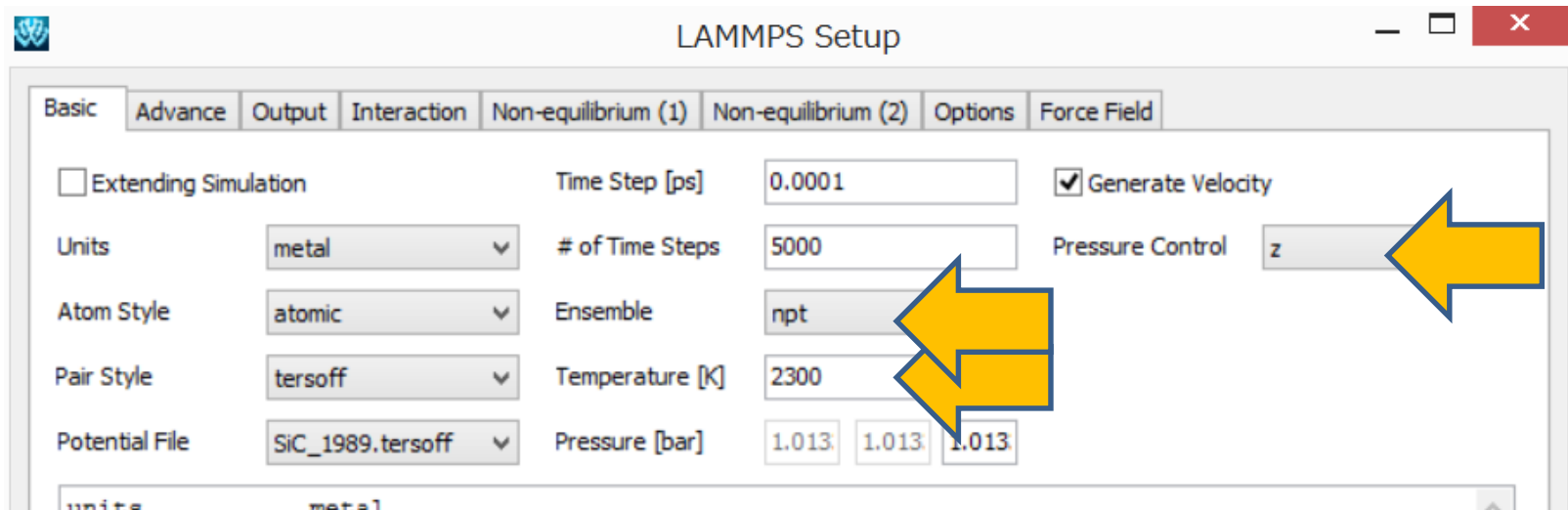
IV. Build of solid-liquid interface system

1. Save as `si_sle.cif`.
2. Click **OK** on the dialog.
3. Click **Cancel** on the **Interface Builder**.
4. Click **red X camera icon**, then interface of this system will be displayed.



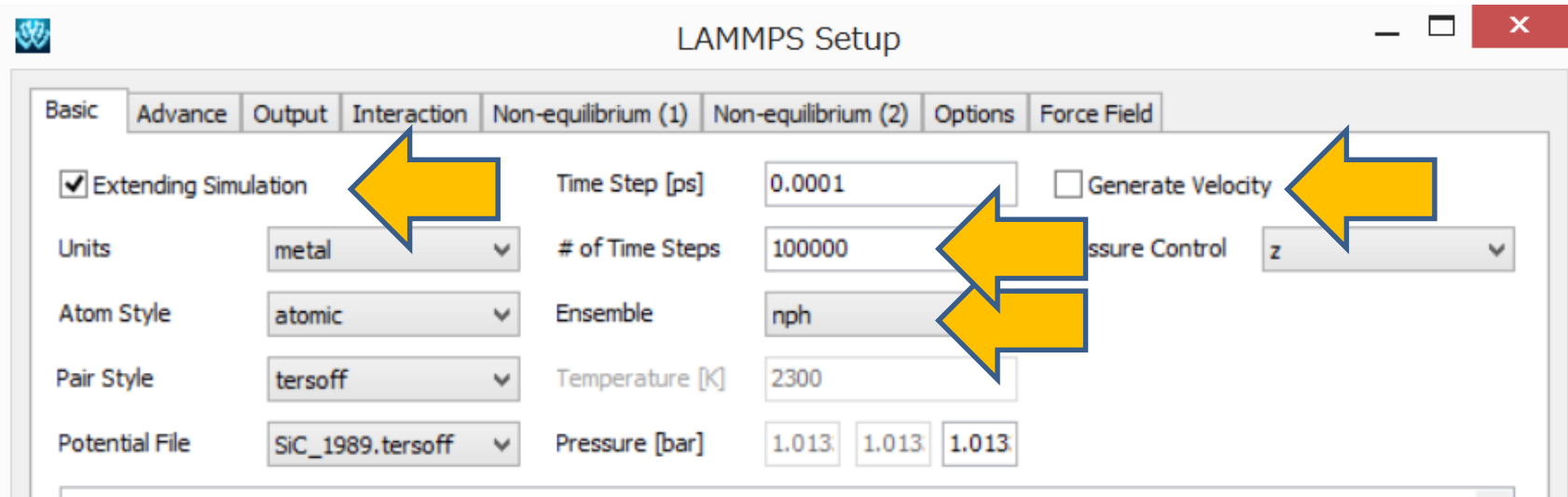
V. Equilibration of interface system

1. Click **MD | LAMMPS | Keywords Setup**.
2. Set **Ensemble** to **npt**, **Temperature** to **2300**, **Pressure Control** to **z**.
3. Click **OK**.
4. Click **MD | LAMMPS | Start LAMMPS**.
5. Save as **si_sle.data**.



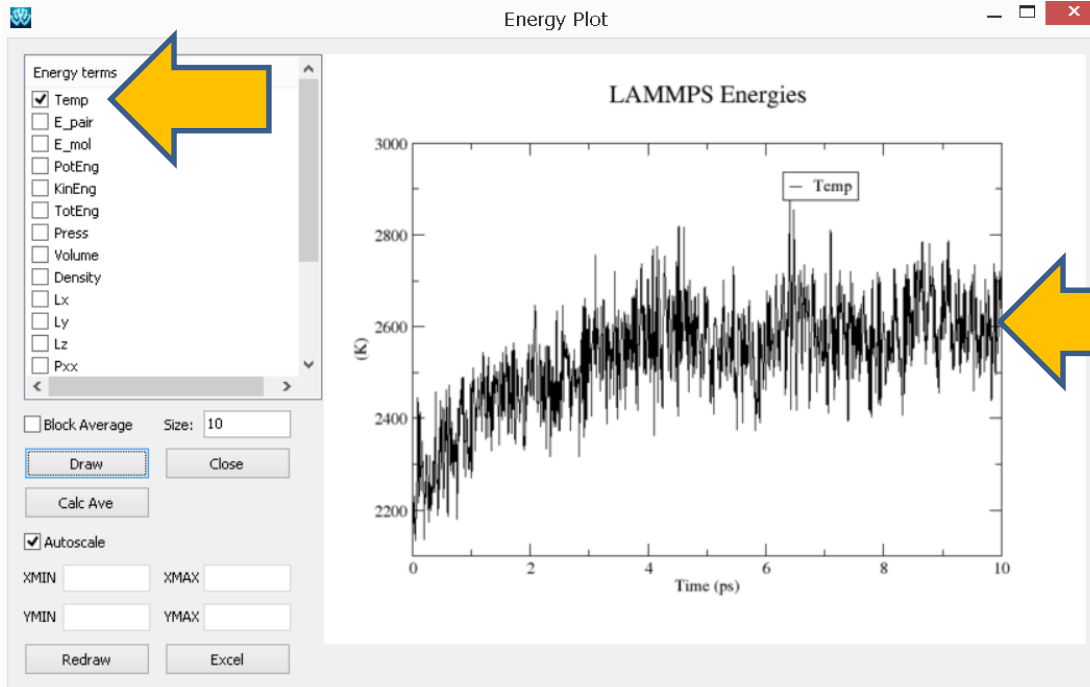
VI. Prediction of melting point

1. After the calculation, click **MD | LAMMPS | Keywords Setup**.
2. Check **Extending Simulation**.
3. Set **# of Time Steps** to 100000, Ensemble to **nph**.
4. Uncheck **Generate Velocity**.
5. Click **OK**.
6. Click **MD | LAMMPS | Start LAMMPS**.



VI. Prediction of melting point

1. After the calculation, click **MD | LAMMPS | Energy Plot**.
2. Open the log file selected by default.
3. Check **Temp**, then click **Draw** to display temperature changes.



The melting point will be the temperature at equilibrium if equilibrium temperature and the final temperature are equivalent (reference below).

The final temperature here was in the vicinity of 2600K. On the other hand, the temperature after equilibration was at 2300K (refer to p.16). According to the statement above, this is not the melting point.

Adopt the final temperature (2600K in this example) as the equilibration temperature and repeat steps II. to VI.

Reference: S. Yoo, X. C. Zeng and J. R. Morris, J. Chem. Phys., 120, 3, (2004), 1654–1656.