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# Winmostar tutorial
## LAMMPS
## Melting point
V7.025

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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.

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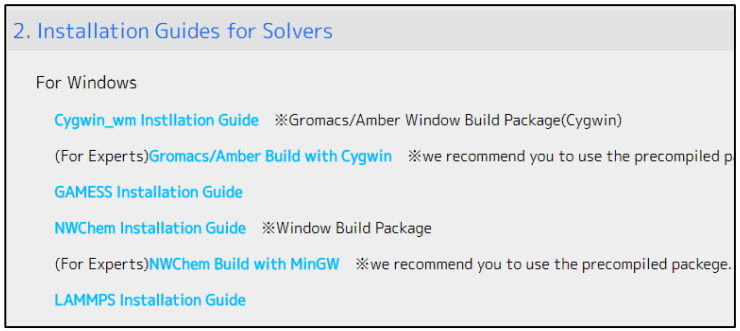
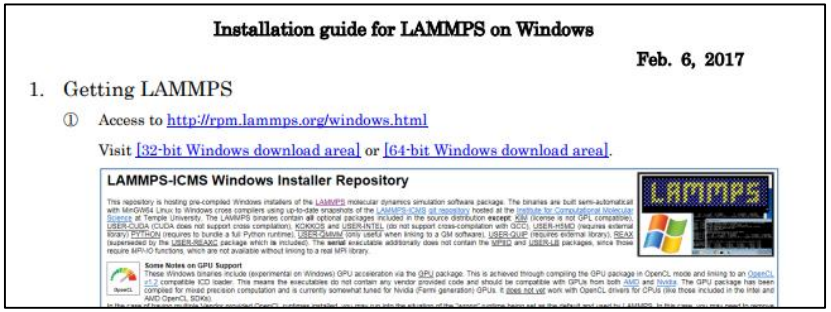
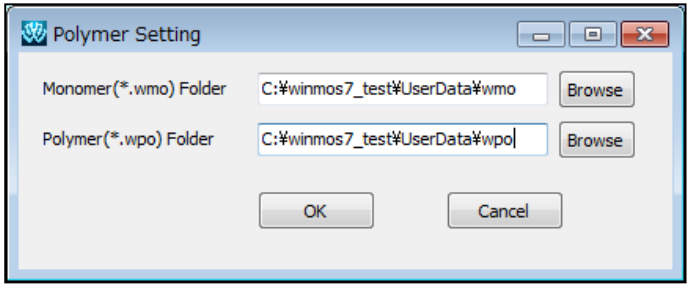
# Configuration

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




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



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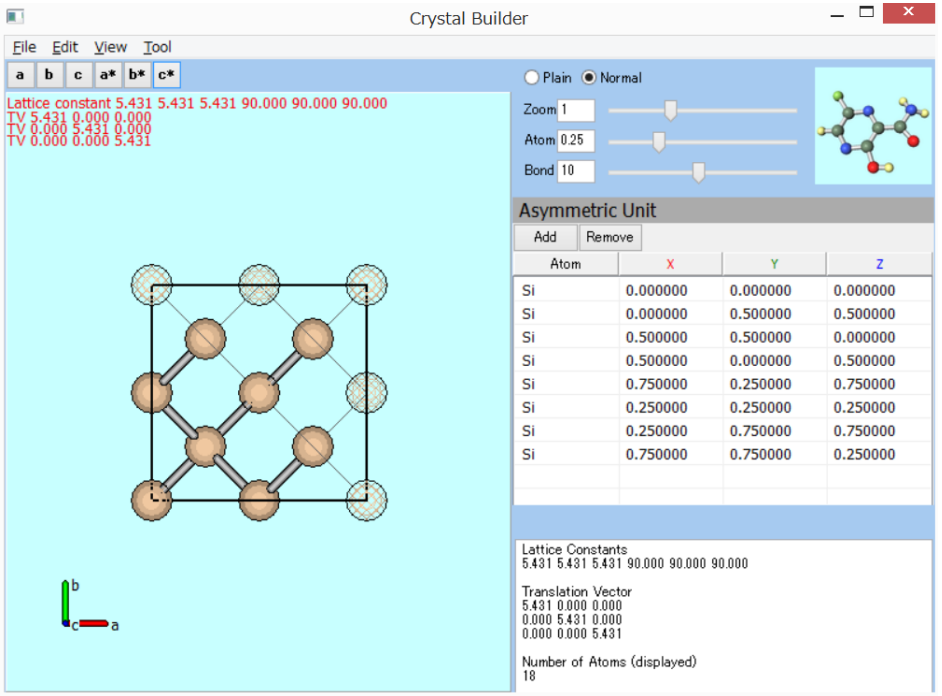
# I. Build solid phase

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)



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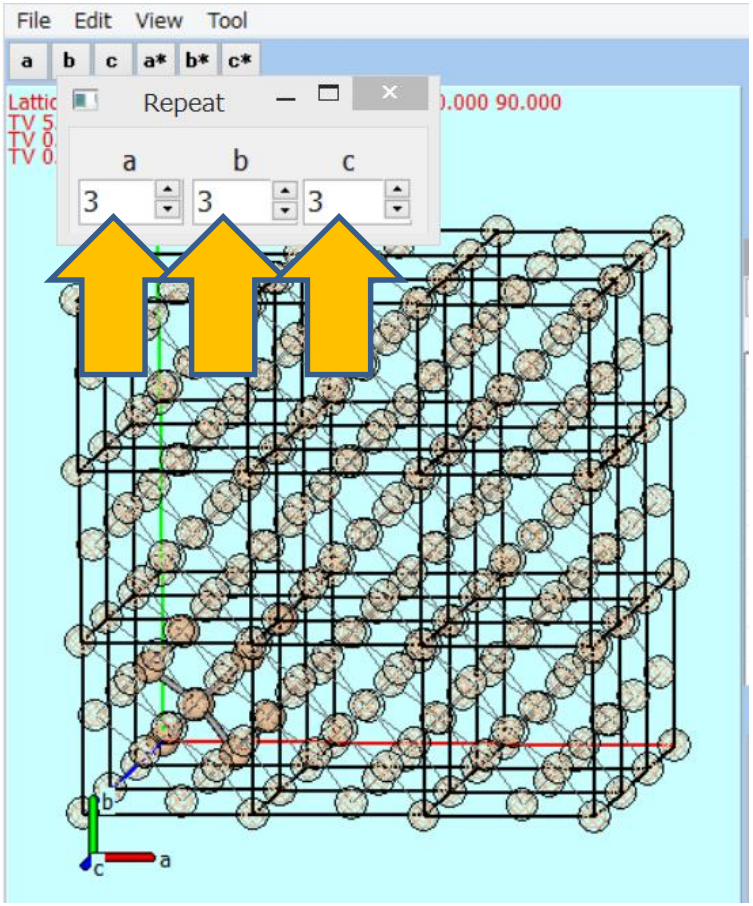
# I. Build solid phase

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



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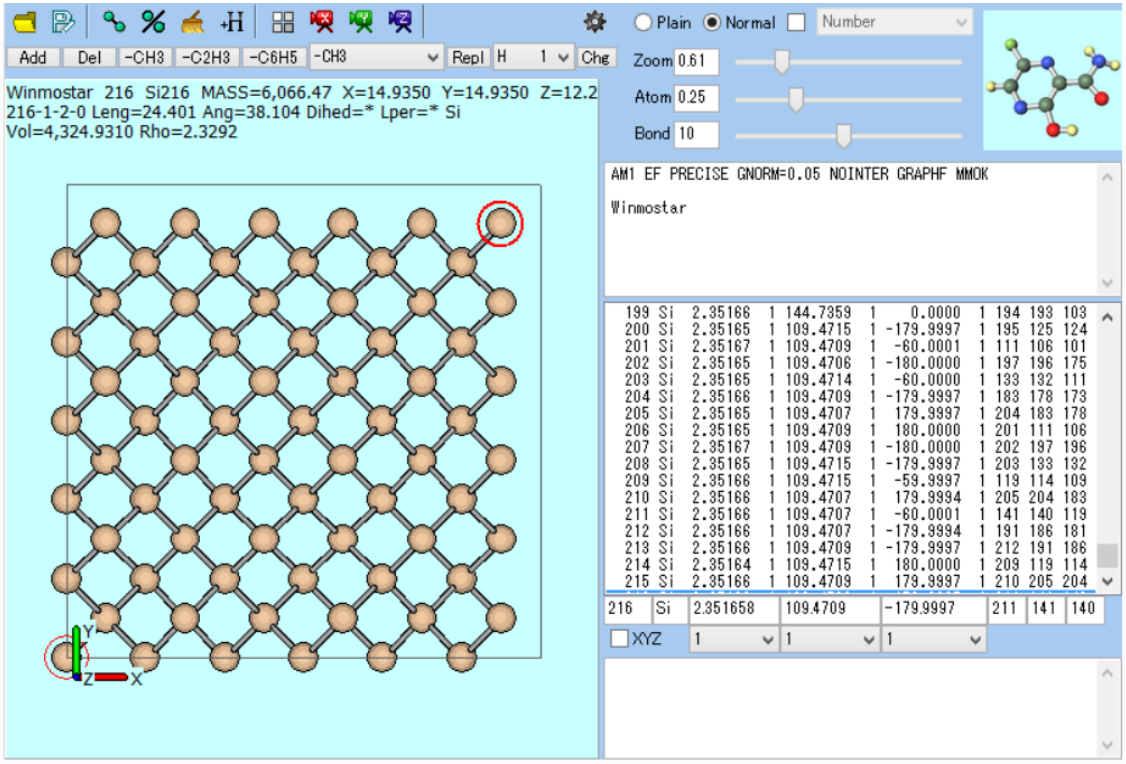
# I. Equilibration of solid phase

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



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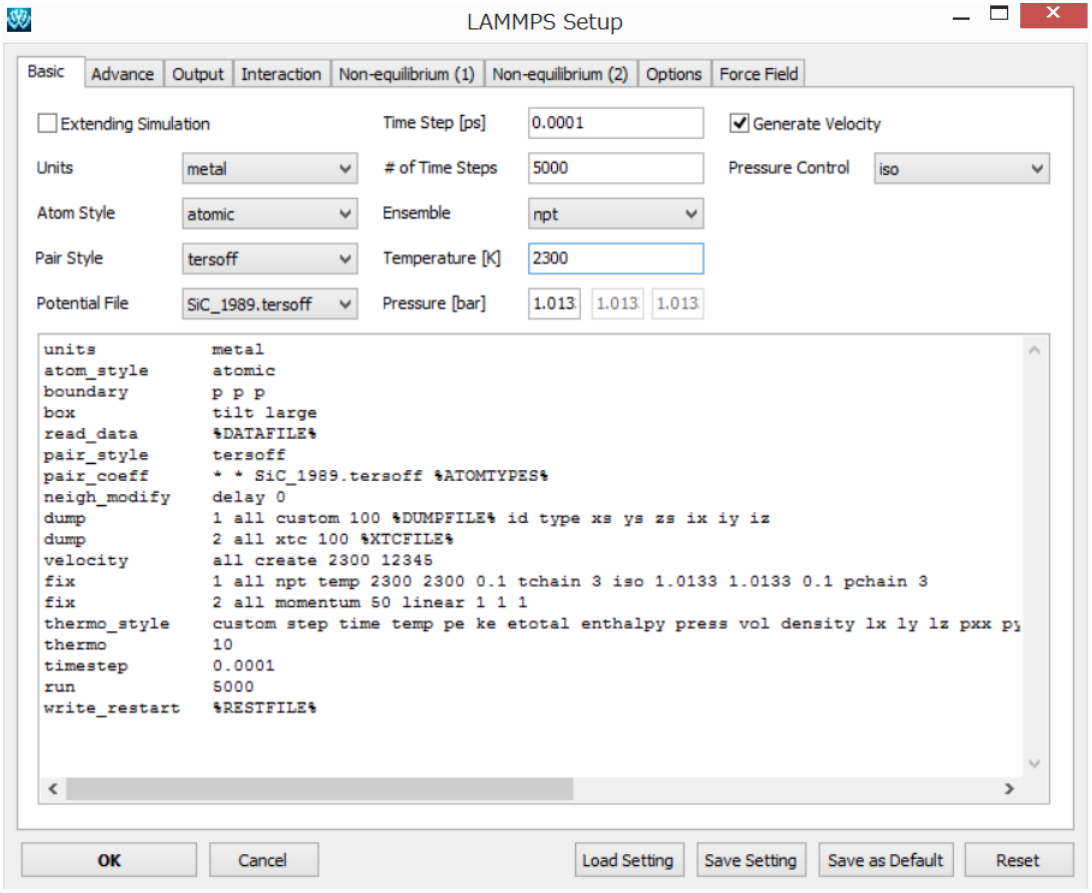
# II. Equilibration of solid phase

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**.



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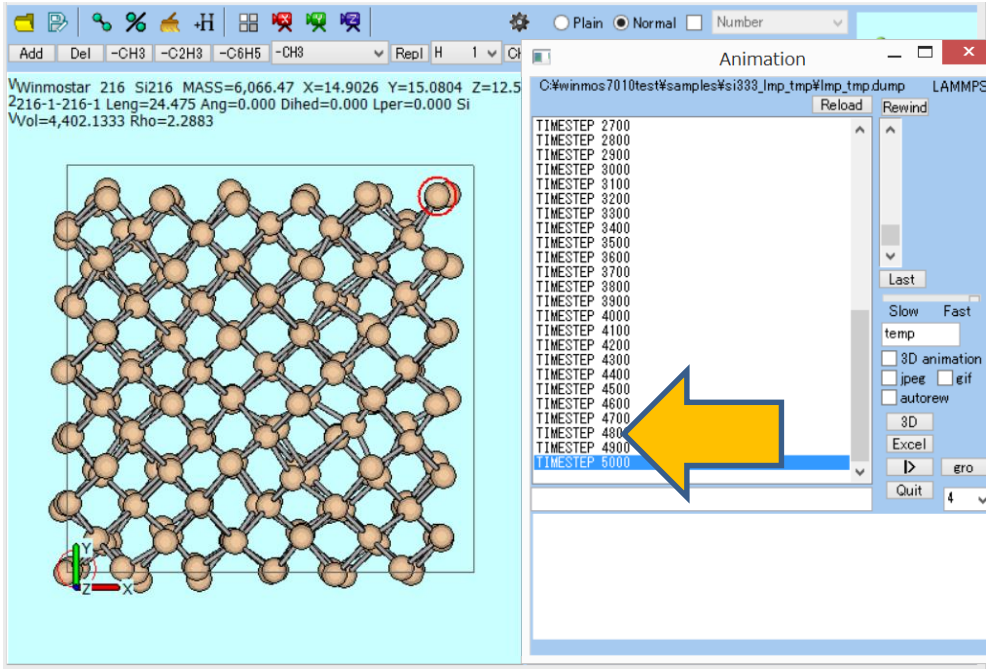
# II. Equilibration of solid phase

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.



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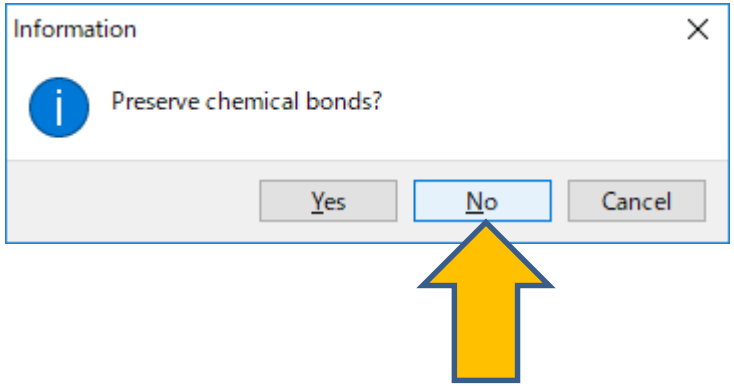
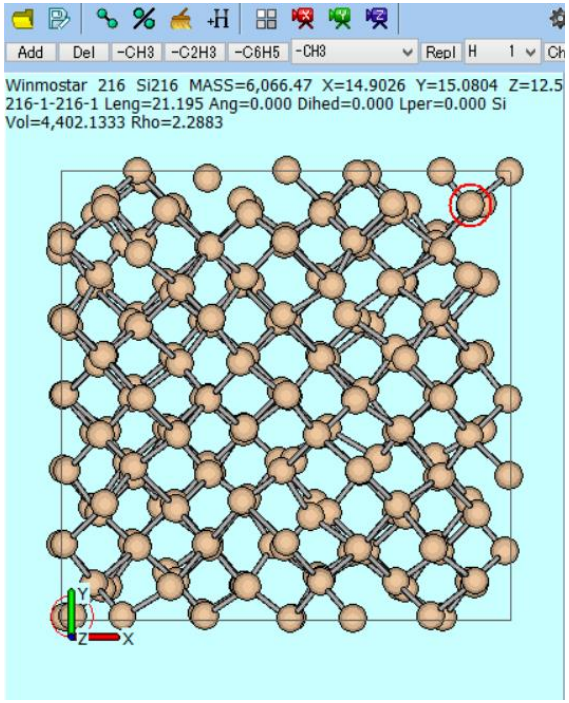
# II. Equilibration of solid phase

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**.



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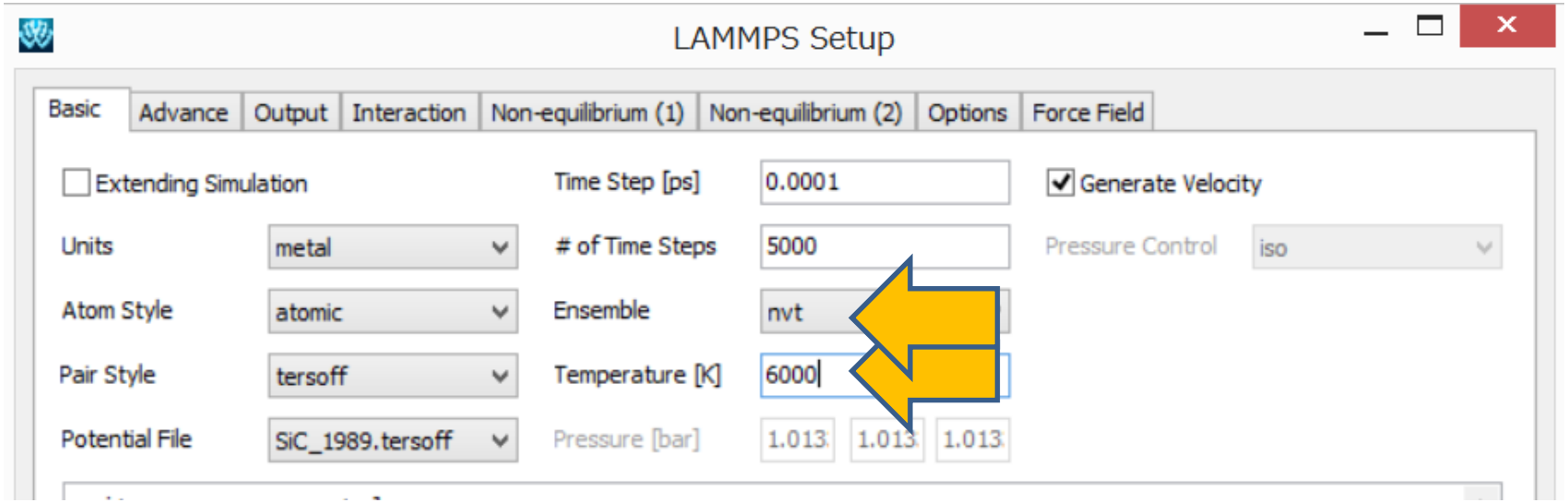
# III. Equilibration of liquid phase

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**.



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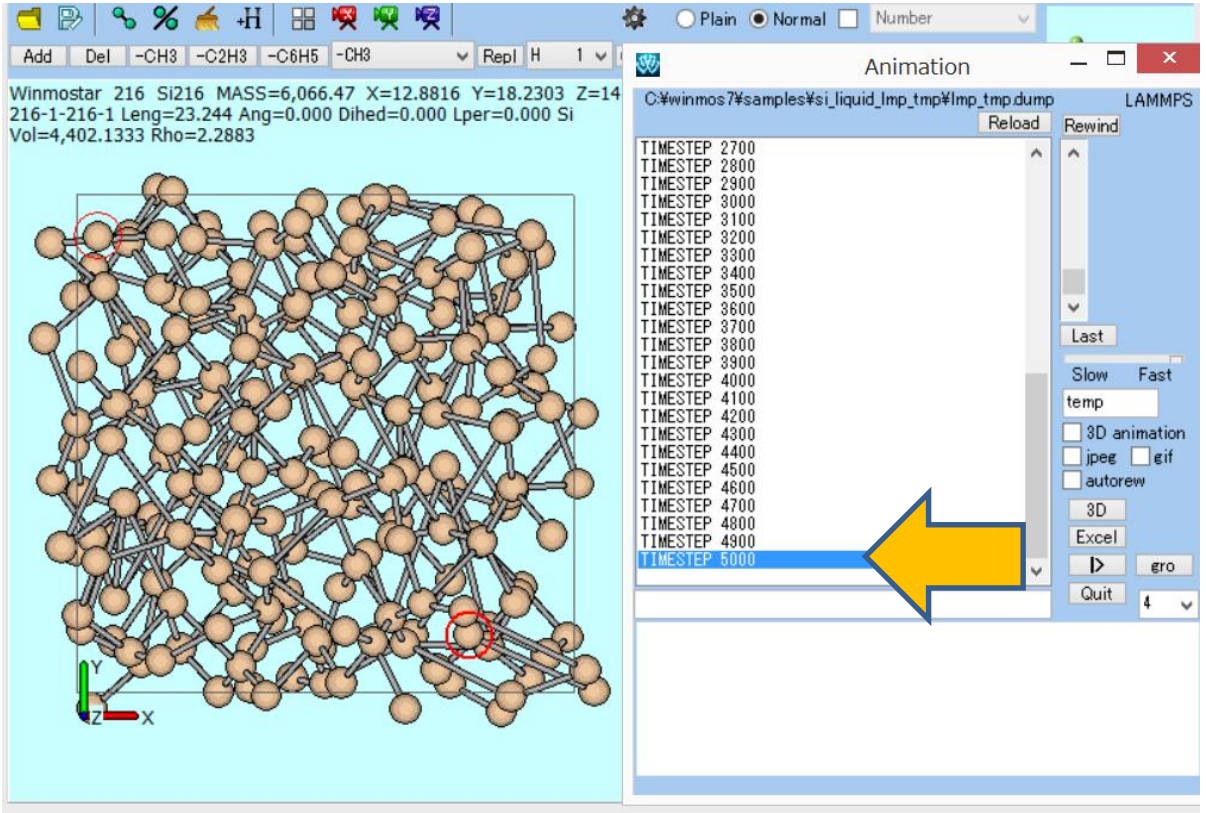
# III. Equilibration of liquid phase

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.



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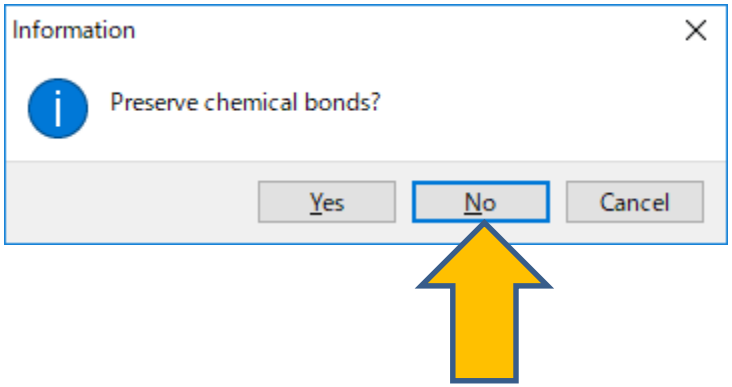
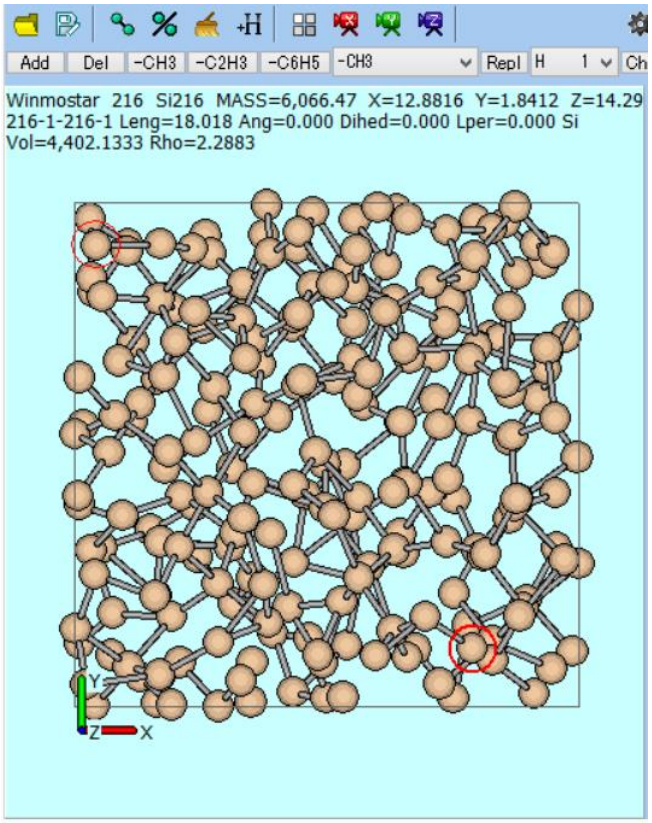
# III. Equilibration of liquid phase

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



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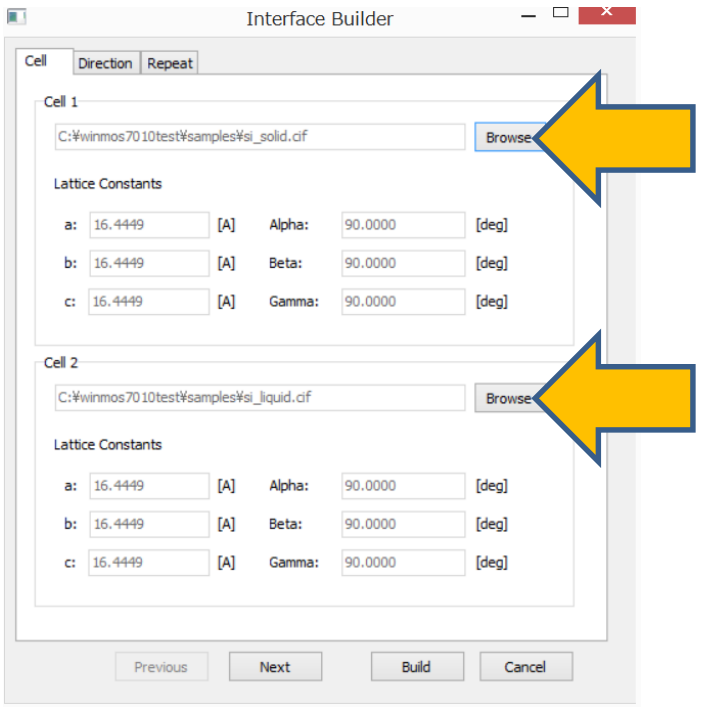
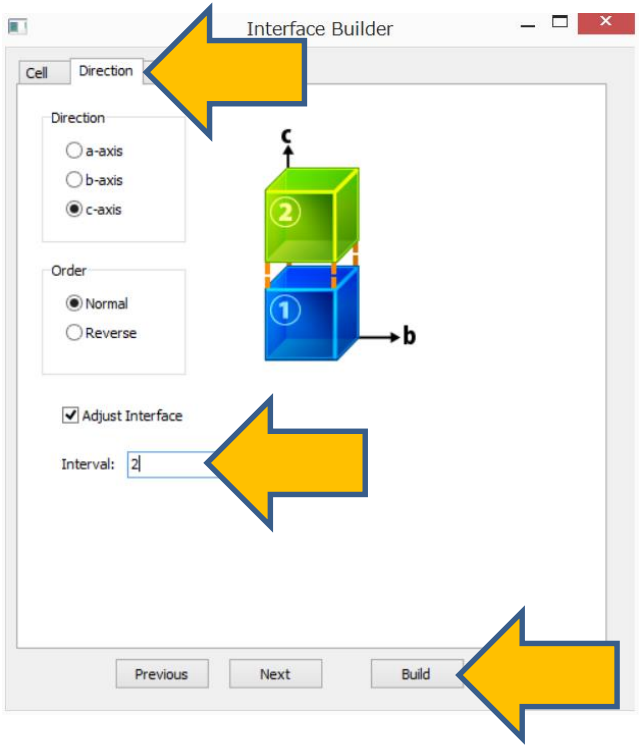
# IV. Build of solid–liquid interface system

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**.



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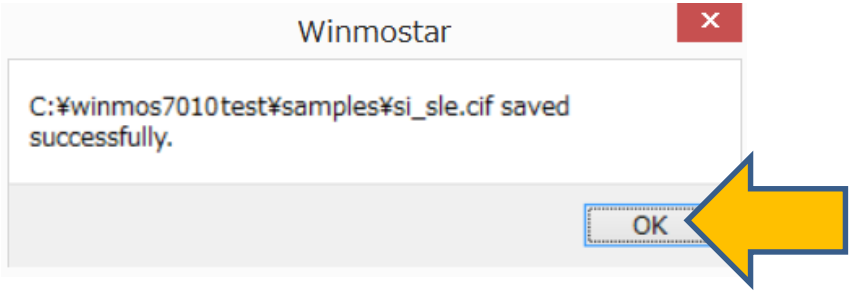
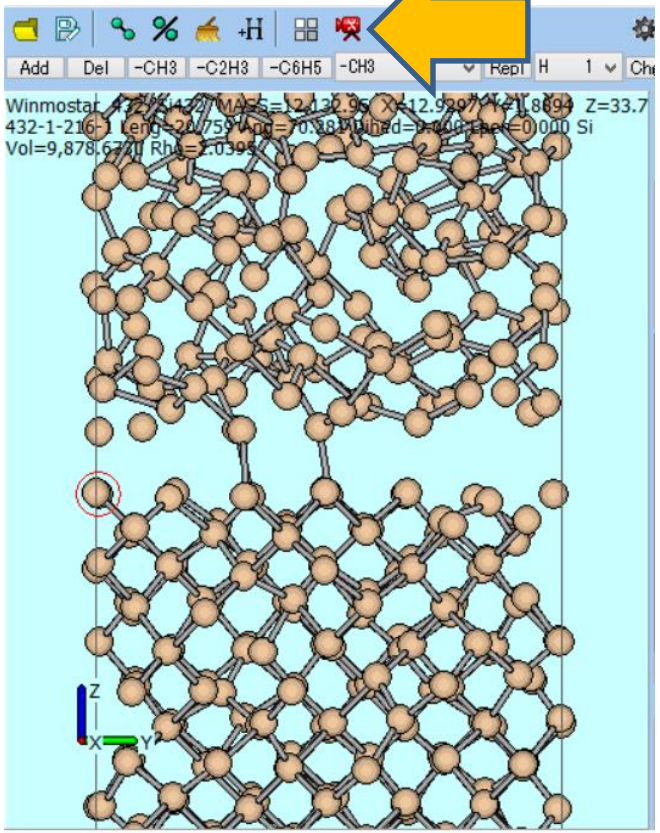
# IV. Build of solid–liquid interface system

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.



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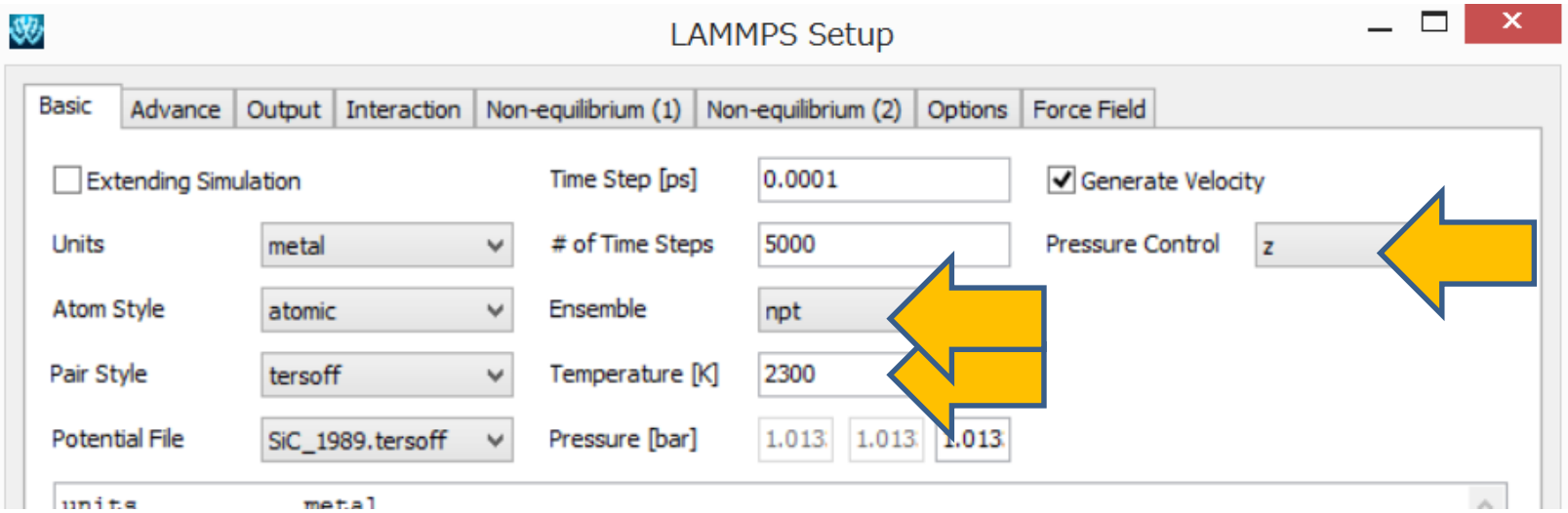
# V. Equilibration of interface system

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**.



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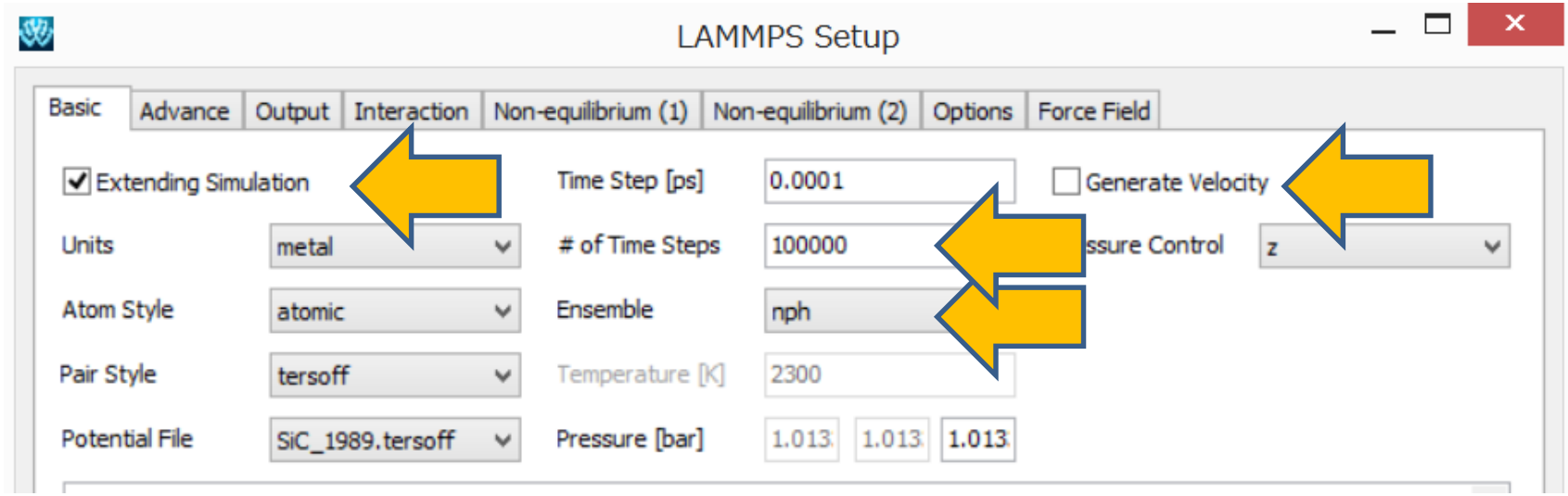
# VI. Prediction of melting point

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**.



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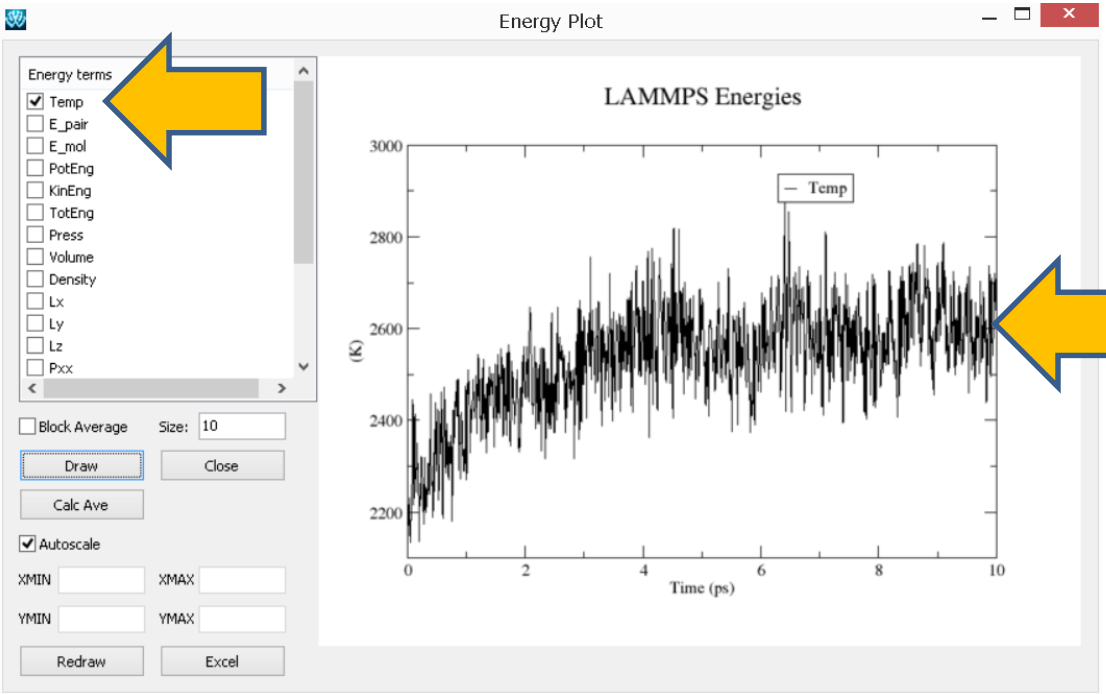
# VI. Prediction of melting point

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.