winmostar tutorial

LAMMPS
Tensile Test Calculation (Solids)

V11.6.5

27 March 2024 X-Ability Co., Ltd.

About This Manual

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - Winmostar Introductory Training Session:This guide only introduces the operation methods of the Basic Tutorial.
  - Winmostar Basic Training Session:We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
  - Individual Training Session:You can freely customize the training content according to your preferences.
- If you are unable to proceed with the operations as outlined in this manual, please first consult Frequently asked questions.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using Contact page. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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Overview

- This tutorial demonstrates the procedure for tensile test calculations of Al crystal.

Note:

- The number of steps required for equilibration depends on the type of material and its initial density.
- The method of interaction calculation, type of force field, size of the supercell, and strain rate all affect the results.

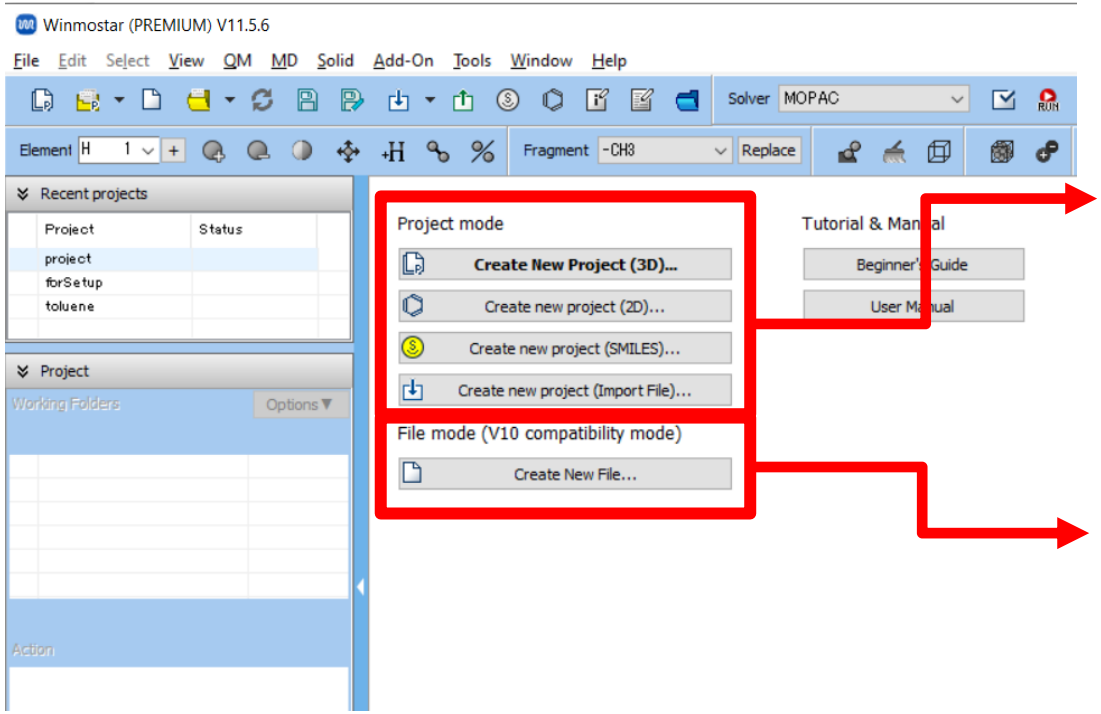
Preference of Operating Environment

- If you are using Winmostar V11.5.0 or later and are on a 64-bit environment, please install and configure CygwinWM version 2023/04/05 or later.
  - The CygwinWM version 2023/04/05 and later includes the recommended version of 64-bit LAMMPS.

- If the above does not apply to you, or if you wish to use a version of LAMMPS other than the recommended version, you will need to separately install and configure the Windows version of LAMMPS.

Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**.
This manual focuses on operations in Project Mode.
For operations in File Mode, please refer to tutorial for version 10.



Project Mode New Features in V11

Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

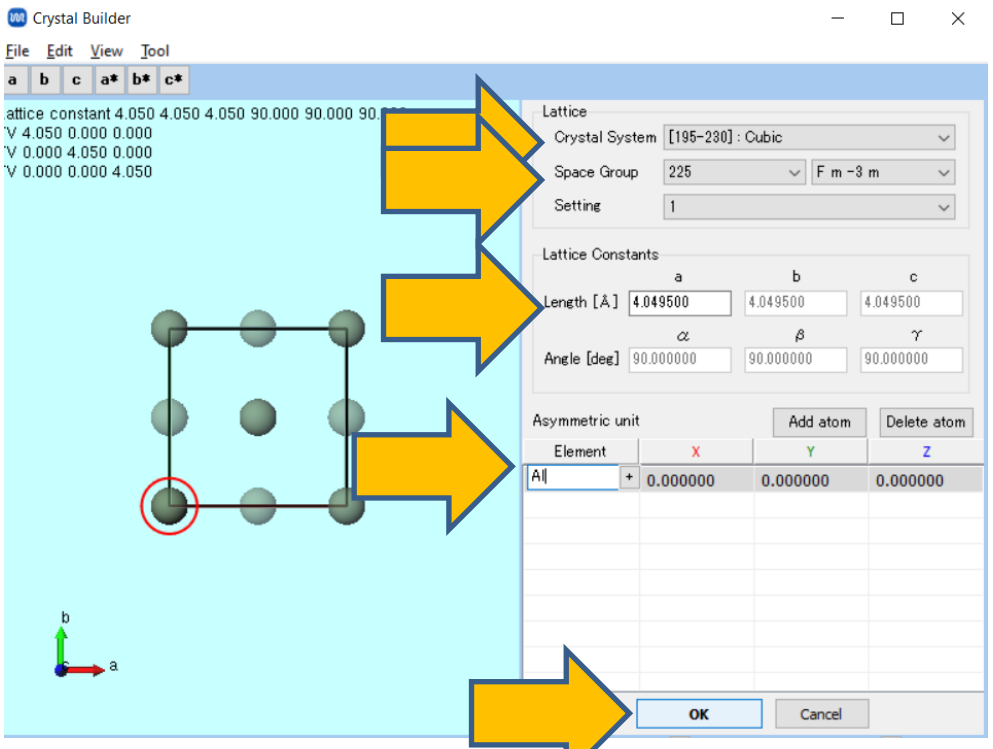
File Mode

Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System

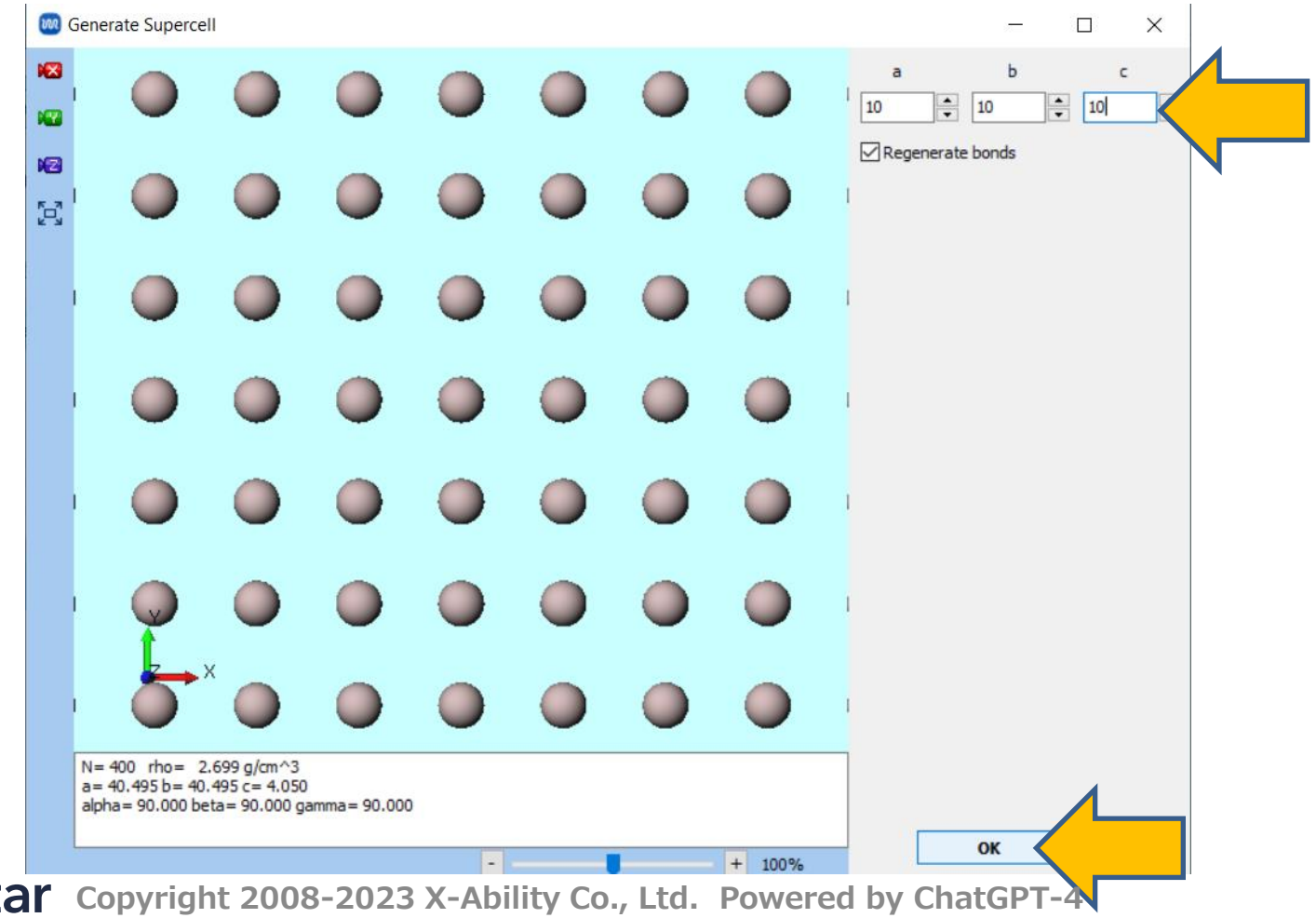
For basic operations, please refer to LAMMPS Basics tutorial.

A. Click **File | New Project**, enter '`al_elong`' in **Project name**, and click **Save**.
B. Click **Solid** | **Crystal Builder**.
C. Change **Crystal System** to '[195-230]: Cubic', **Space Group** to '225 (Fm-3m)', **a** to '4.0495', and **Element** in **Asymmetric unit** to 'Al'.
D. Click **OK**.



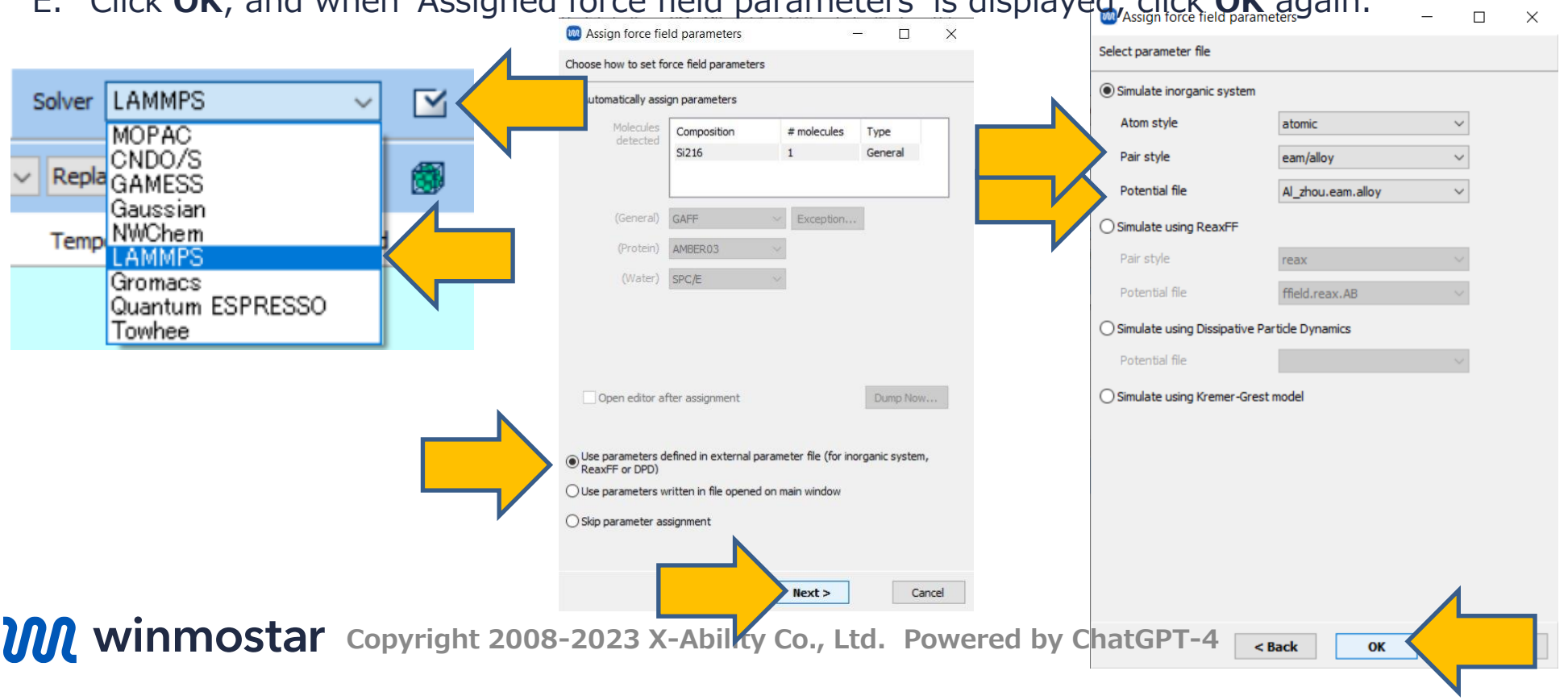
A. Modeling of the System

A. Click **Solid | Generate Supercell**.
B. Change **a, b, c** all to '10' and click **OK**.



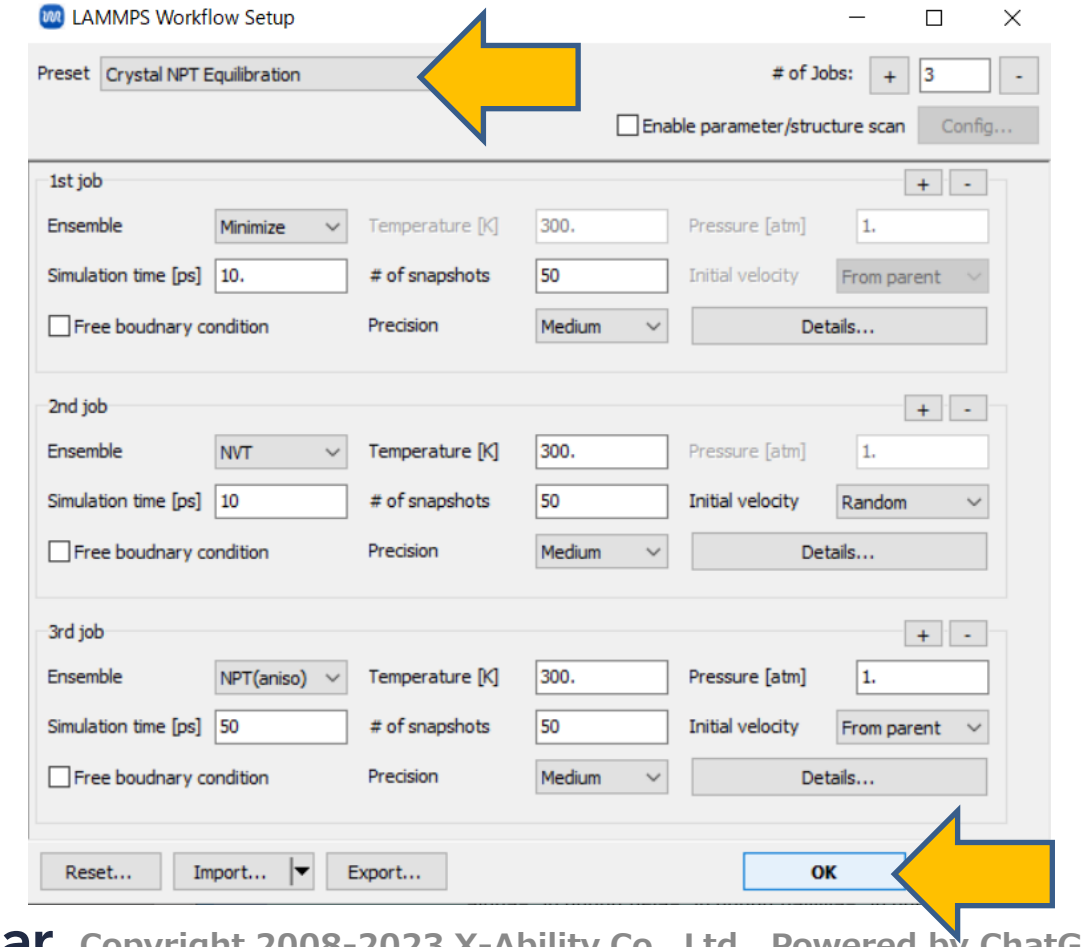
B. Execution of Calculation（Equilibration）

A. Select **LAMMPS** from **Solver** and open **(Keyword Setup)**.
B. If prompted 'Some molecules do not have charges. Do you want to assign charges now?' click **No**.
C. Choose **Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)** and click **Next**.
D. Change **Pair Style** to 'eam/alloy' and **Potential File** to 'Al_zhou.eam.alloy'.
E. Click **OK**, and when 'Assigned force field parameters' is displayed, click **OK** again.



B. Execution of Calculation（Equilibration）

A. Change **Preset** to 'Crystal NPT Equilibration'.
B. Click **OK**, and after making appropriate settings in **Job Setting** window, click **Run**.

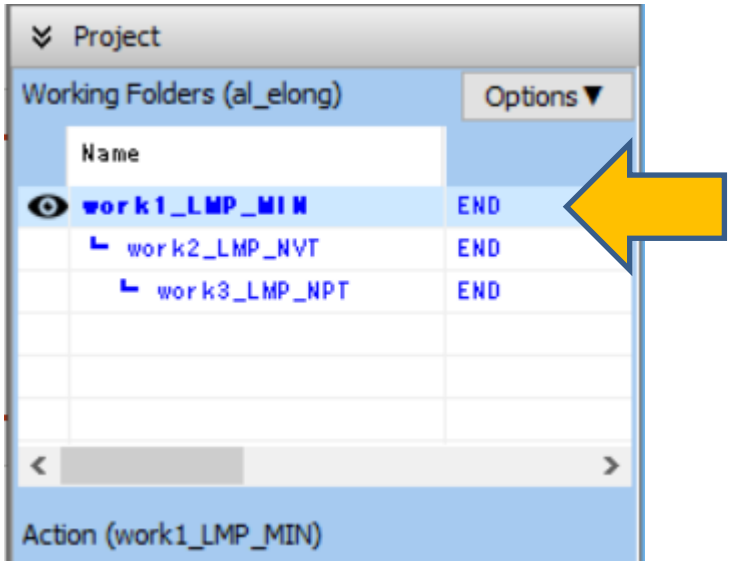


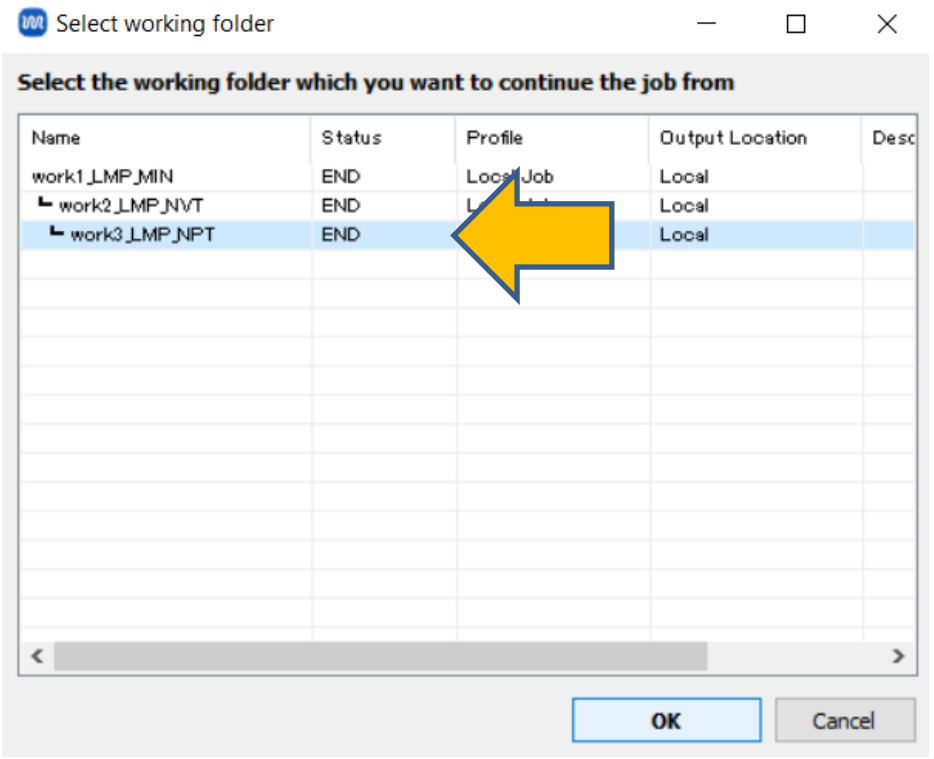
C. Execution of Calculation（Main Calculation）

A. Once **the status** of **the work folders** from work1_LMP_MIN to work3_LMP_NPT changes to **END** or **END(-)**, click **(Workflow Setup)**.

B. If prompted with 'Do you want to continue from previous run?', click **Yes**.

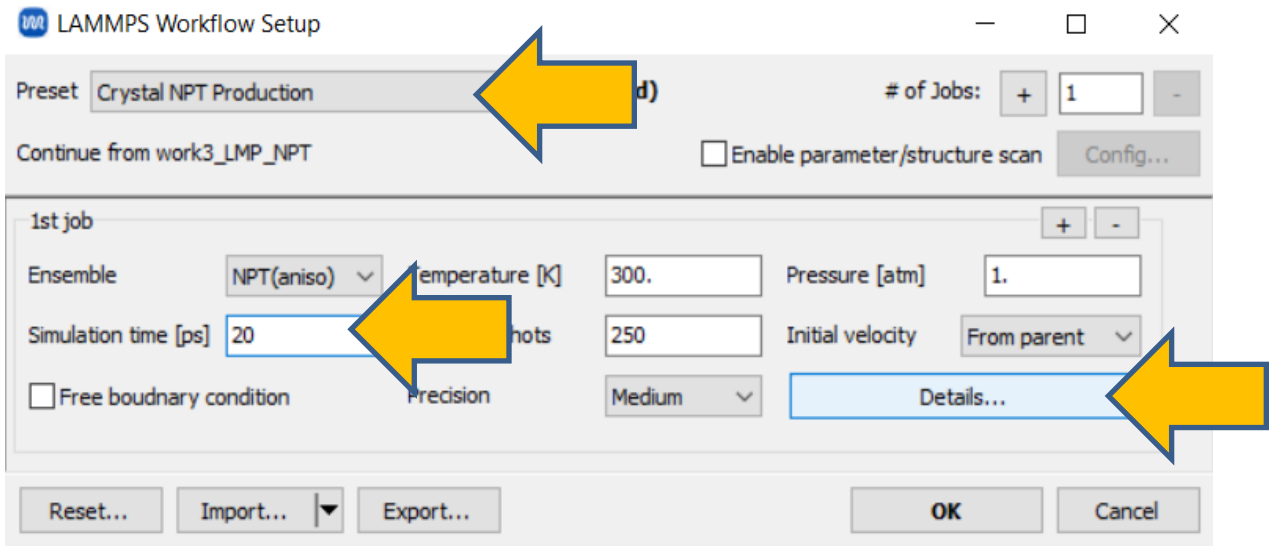
C. Select work3_LMP_NPT and click **OK**.





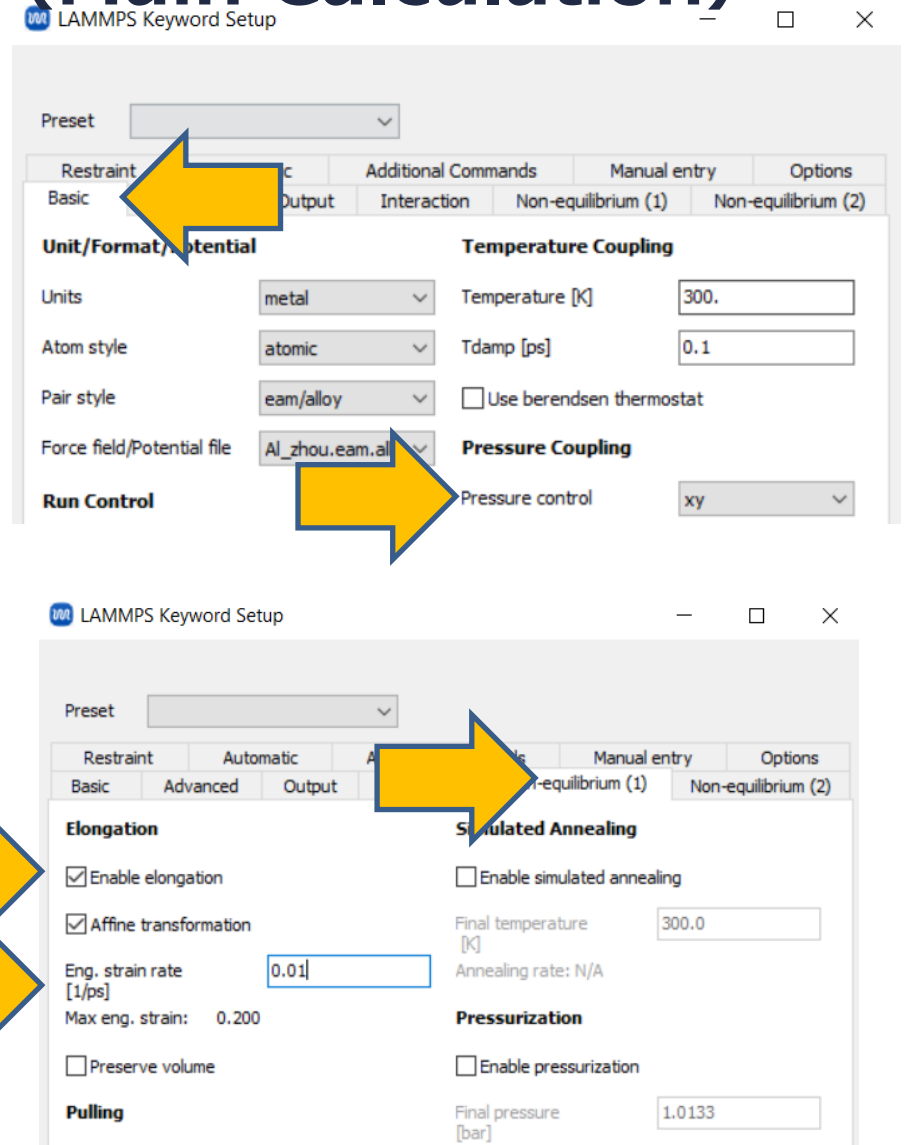
C. Execution of Calculation（Main Calculation）

A. Change **Preset** to 'Crystal NPT Production'.
B. Change **Simulation time** for **1st job** to '20'.
C. Click **Details…**.



C. Execution of Calculation (Main Calculation)

A. In **LAMMPS Keyword Setup** window, under **Basic tab**, change **Pressure control** to 'xy'.
B. Move to **Non-equilibrium(1)** tab and change the settings as follows:
   A. Check **Enable elongation**.
   B. Change **Eng. Strain Rate** to '0.01'.
C. Click **OK** to close **LAMMPS Keyword Setup** window.
D. Click **OK** in **LAMMPS Workflow Setup** window.
E. In **Job Setting** window, adjust settings as necessary and click **Run**.

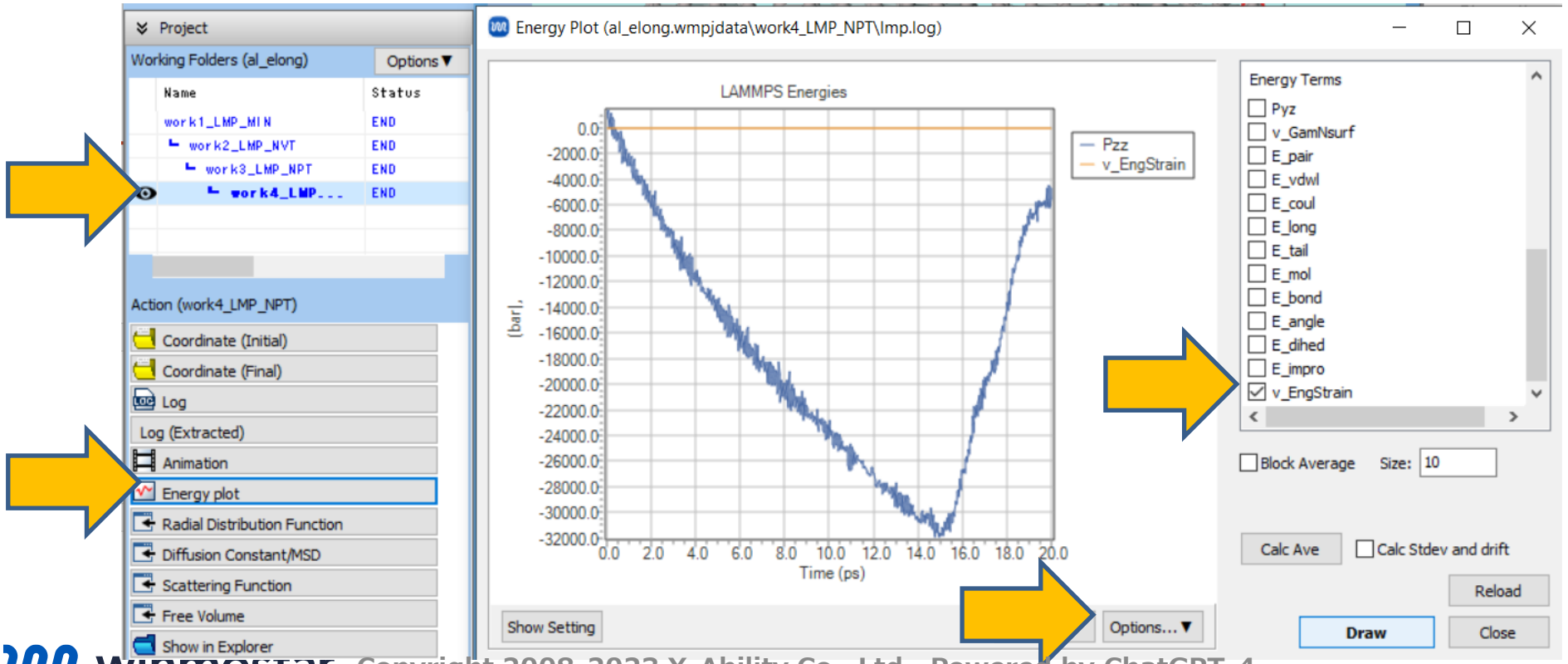


D. Analysis of Results

A. Once **the status** of **the work folder** 'work4_LMP_NPT' changes to **END** or **END(-)**, click on 'work4_LMP_NPT' and then click **Energy plot** in **Action**.

B. In **Energy Terms**, check **Pzz** and **EngStrai**, then click **Draw**, followed by clicking **Options | Export csv & Open Excel**.

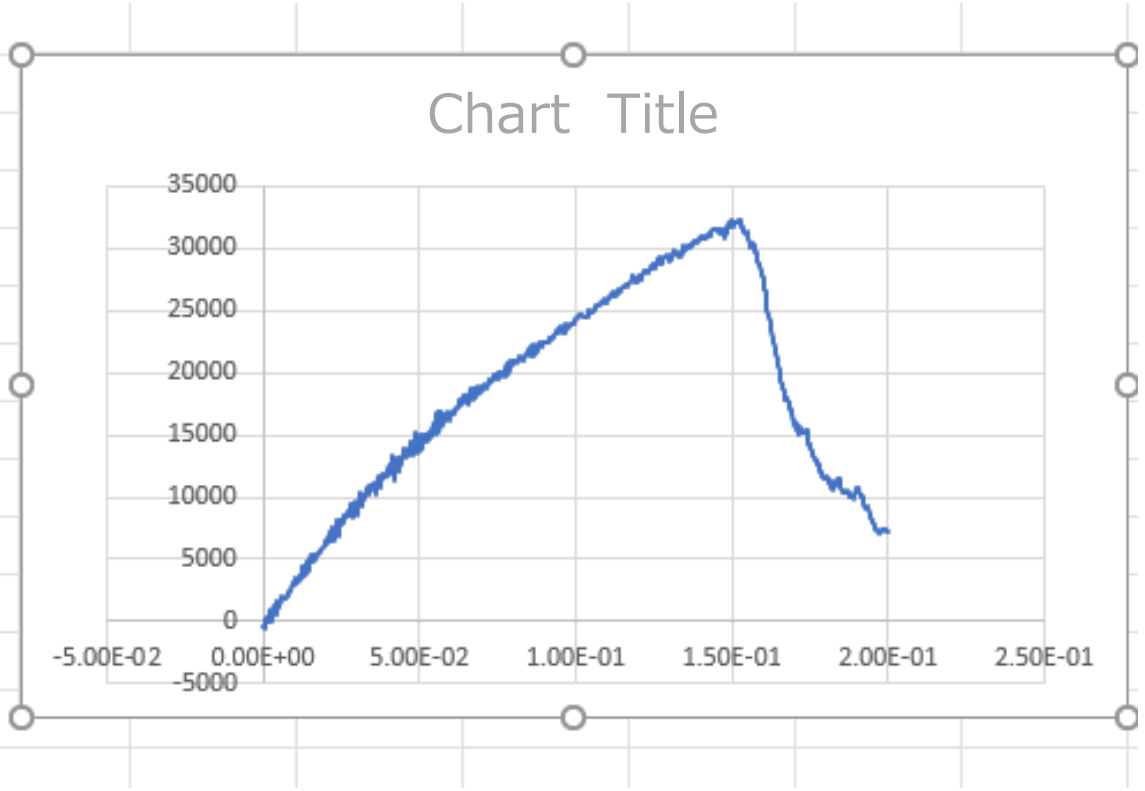
C. Click **Save** in **Save As** dialog.



D. Analysis of Results

A. Open the CSV file, plot the third column (engineering strain) on the x-axis and the second column multiplied by -1 (Pzz) on the y-axis to generate the stress-strain curve.

48	-8228.36	0.1948	8228.356
.5	-8244.8	1.95E-01	8244.802
52	-8209.67	0.1952	8209.67
54	-8054.42	0.1954	8054.425
56	-7850.76	1.96E-01	7850.764
58	-7644.79	0.1958	7644.786
.6	-7458.95	0.196	7458.945
62	-7466.25	1.96E-01	7466.25
64	-7497.5	0.1964	7497.5
66	-7379.35	0.1966	7379.348
68	-7314.43	1.97E-01	7314.43
.7	-7253.35	0.197	7253.351
72	-7114.64	0.1972	7114.639
74	-7109.18	1.97E-01	7109.182



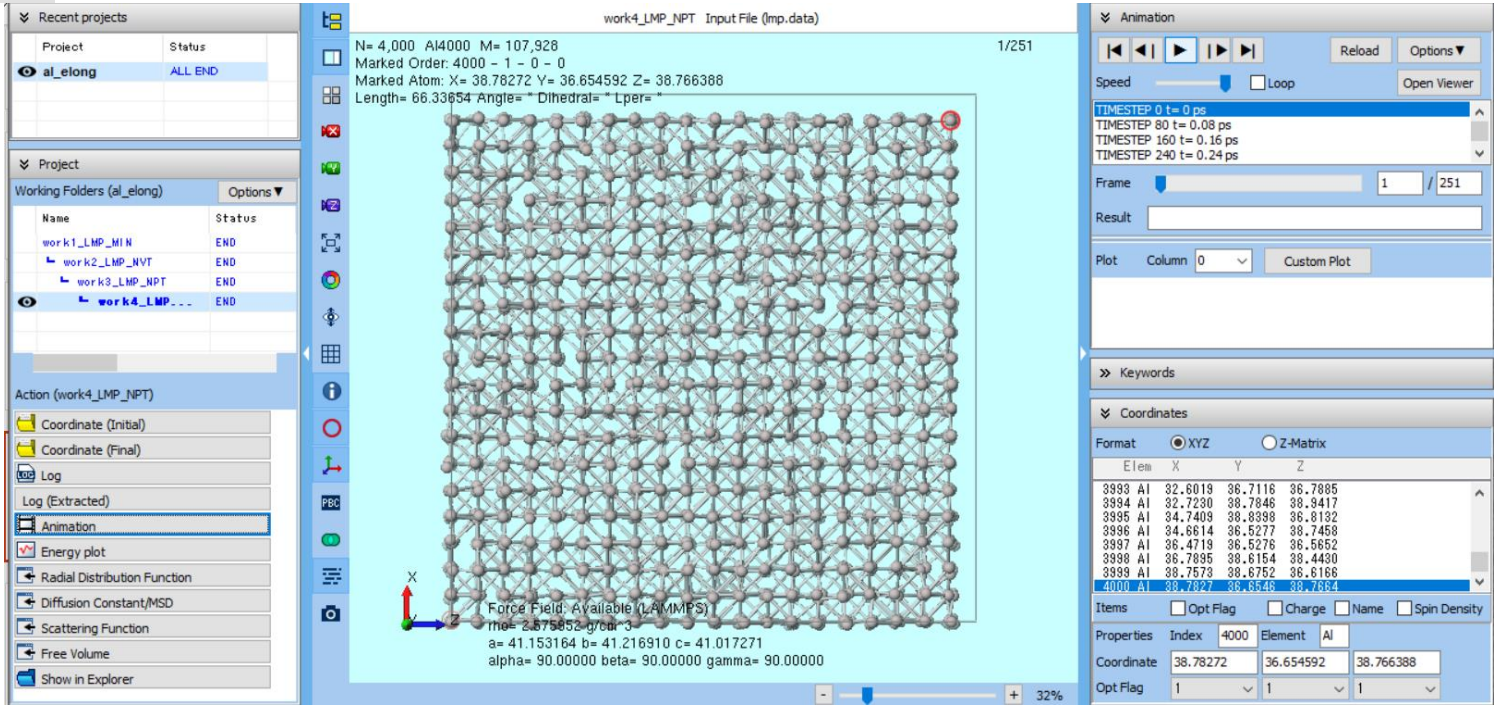
D. Analysis of Results

A. Return to Winmostar and close **Energy Plot** window by clicking **Close**.

B. Click 'work4_LMP_NPT' folder in **Working Folders**, then click  **Animation** in **Action**. After a few seconds of processing, an area for controlling the animation will appear.

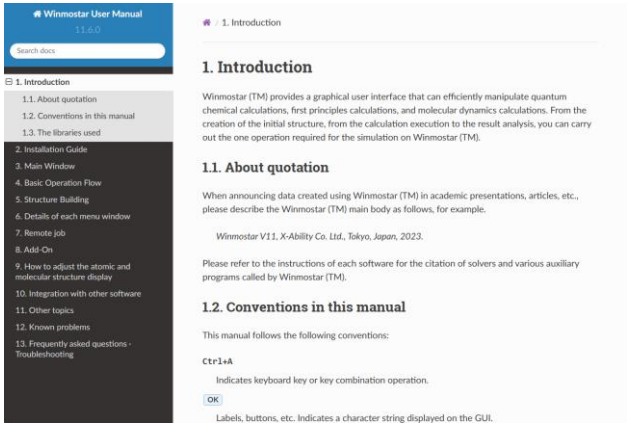
C. Click  **(Align View to Y-Axis)**.

D. Click  **(Play/Pause)** to observe the animation.



Finally

- For detailed information on each feature, please refer to Winmostar User Manual.



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Scenes from Winmostar Training Session

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