Molecular Dynamics Simulation of the $Zr_{47}Cu_{46}Al_7$ Metallic Glass

Developed and Implemented by Roozbeh Aghabarari

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1. LAMMPS Code

```
# Molecular Dynamics Simulation of the Zr47Cu46Al7 Metallic Glass
#                            Coded by
#                        Roozbeh Aghabarari
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#
# Initialization
units           metal
dimension       3
boundary        p p p
atom_style      atomic

# Define the simulation box and atoms
region          simbox block 0 30 0 30 0 30 units box
create_box      3 simbox
create_atoms    2 random 1000 5165 simbox

# Grouping and setting atom types
group           grp_Cu type 2
set             group grp_Cu type/fraction 3 0.478 12393
set             group grp_Cu type/fraction 1 0.079 12393

# Define masses for each atom type
mass            1 26.98  # Al
mass            2 63.54  # Cu
mass            3 91.22  # Zr

# Set potential style and coefficients
pair_style      eam/alloy
pair_coeff      * * ZrCuAl.lammps.eam Al Cu Zr

# Simulation settings
timestep        0.001
thermo          10000
thermo_style    custom step temp ke pe etotal

# Energy minimization
min_style       cg
minimize        0.01 0.01 10000 10000

# Resetting timestep and velocity initialization
reset_timestep  0
velocity        all create 300 65416541 dist uniform
```

```
# First phase: Heating from 300 K to 2100 K
fix             heating all npt temp 300 2100 0.1 iso 1 1 1
dump            phase1 all xyz 100 Melting.xyz
dump_modify     phase1 element Al Cu Zr
run             1000000

# Equilibrate at 2100 K
undump          phase1
unfix           heating
fix             equil_highT all npt temp 2100 2100 0.1 iso 1 1 1
dump            phase2 all xyz 100 2100Equilibrium.xyz
dump_modify     phase2 element Al Cu Zr
run             1000000

# Second phase: Cooling from 2100 K to 300 K
undump          phase2
unfix           equil_highT
reset_timestep  0
fix             cooling all npt temp 2100 300 0.1 iso 1 1 1
dump            phase3 all xyz 100 Cooling.xyz
dump_modify     phase3 element Al Cu Zr
run             1800000

# Equilibration at 300 K
undump          phase3
unfix           cooling
fix             equil_roomT all npt temp 300 300 0.1 iso 1 1 1
dump            phase4 all xyz 100 300Equilibrium.xyz
dump_modify     phase4 element Al Cu Zr
run             1000000
```

1.1. Description

1.1.1. Initialization

- `units  metal`
  → Defines the unit style for metallic systems.

- `dimension  3`
  → Specifies 3D simulation.

- `boundary  p p p`
  → Applies periodic boundary conditions in all three directions.

- `atom_style  atomic`
  → Uses a basic atom style without additional attributes.

1.1.2. Define the simulation box and atoms

- `region  simbox block 0 30 0 30 0 30 units box`
  → Defines a simulation box from (0,0,0) to (30,30,30).

- `create_box 3 simbox`
  → Initializes the simulation box for three atom types.

- `create_atoms 2 random 1000 5165 simbox`
  → Randomly places 1000 atoms of type 2 (Cu) within the simulation box.

1.1.3. Grouping and setting atom types

- `group grp_Cu type 2`
  → Creates a group named grp_Cu for atoms of type 2.

- `set group grp_Cu type/fraction 3 0.478 12393`
  → Converts 47.8% of Cu atoms into type 3 (Zr).

- `set group grp_Cu type/fraction 1 0.079 12393`
  → Converts 7.9% of Cu atoms into type 1 (Al).

1.1.4. Define masses for each atom type

- `mass 1 26.98`
  → Sets the mass of atom type 1 (Al) to 26.98 atomic mass units.

- `mass 2 63.54`
  → Sets the mass of atom type 2 (Cu) to 63.54 atomic mass units.

- `mass 3 91.22`
  → Sets the mass of atom type 3 (Zr) to 91.22 atomic mass units.

1.1.5. Set potential style and coefficients

- `pair_style eam/alloy`
  → Uses the Embedded Atom Method (EAM) for metallic interactions.

- `pair_coeff * * ZrCuAl.lammps.eam Al Cu Zr`
  → Associates the EAM potential file with the three elements.

1.1.6. Simulation settings

- `timestep 0.001`
  → Sets the integration timestep to 0.001 ps.

- `thermo 10000`
  → Outputs thermodynamic data every 10000 steps.

- `thermo_style custom step temp ke pe etotal`
  → Customizes the thermodynamic output to include step number, temperature, kinetic energy, potential energy, and total energy.

1.1.7. Energy minimization

- `min_style cg`
  → Uses the conjugate gradient algorithm for energy minimization.

- `minimize 0.01 0.01 10000 10000`
  → Minimizes system energy with specified tolerances and iteration limits.

1.1.8. Resetting timestep and velocity initialization

- `reset_timestep 0`
  → Resets the timestep counter.

- `velocity all create 300 65416541 dist uniform`
  → Initializes atomic velocities corresponding to 300 K.

1.1.9. First phase: Heating from 300 K to 2100 K

- `fix heating all npt temp 300 2100 0.1 iso 1 1 1`
  → Applies a Nose-Hoover thermostat and barostat to heat the system from 300 K to 2100 K under constant pressure.

- `dump phase1 all xyz 100 Melting.xyz`
  → Dumps atomic coordinates to a file every 100 steps during the heating phase.

- `dump_modify phase1 element Al Cu Zr`
  → Modifies the dump file to include element names.

- `run 1000000`
  → Runs the simulation for 1000000 timesteps.

1.1.10. Equilibrate at 2100 K

- `undump phase1`
  → Stops the dump of coordinates from the heating phase.

- `unfix heating`
  → Removes the heating fix.

- `fix equil_highT all npt temp 2100 2100 0.1 iso 1 1 1`
  → Maintains the system at 2100 K under constant pressure.

- `dump phase2 all xyz 100 2100Equilibrium.xyz`
  → Dumps atomic coordinates to a file every 100 steps during the equilibration phase.

- `dump_modify phase2 element Al Cu Zr`
  → Modifies the dump file to include element names.

- `run 1000000`
  → Runs the simulation for 1000000 timesteps.

1.1.11. Second phase: Cooling from 2100 K to 300 K

- `undump phase2`
  → Stops the dump of coordinates from the equilibration phase.

- `unfix equil_highT`
  → Removes the equilibration fix.

- `reset_timestep 0`
  → Resets the timestep counter to 0.

- `fix cooling all npt temp 2100 300 0.1 iso 1 1 1`
  → Applies a Nose-Hoover thermostat and barostat to cool the system from 2100 K to 300 K under constant pressure.

- `dump phase3 all xyz 100 Cooling.xyz`
  → Dumps atomic coordinates to a file every 100 steps during the cooling phase.

- `dump_modify phase3 element Al Cu Zr`
  → Modifies the dump file to include element names.

- `run 1800000`
  → Runs the simulation for 1800000 timesteps.

1.1.12. Equilibration at 300 K

- `undump phase3`
  → Stops the dump of coordinates from the cooling phase.

- `unfix cooling`
  → Removes the cooling fix.

- `fix equil_roomT all npt temp 300 300 0.1 iso 1 1 1`
  → Maintains the system at 300 K under constant pressure.

- `dump phase4 all xyz 100 300Equilibrium.xyz`
  → Dumps atomic coordinates to a file every 100 steps during the room temperature equilibration phase.

- `dump_modify phase4 element Al Cu Zr`
  → Modifies the dump file to include element names.

- `run 1000000`
  → Runs the simulation for 1000000 timesteps.

The first section of the input script defines essential simulation parameters such as dimensionality, boundary conditions, and atomic style. Then, 1000 atoms are randomly positioned, and their types are adjusted to match the target atomic percentages for the metallic glass: approximately 7% Al, 47% Zr, and 46% Cu. These settings result in a representative model of $Zr_{47}Cu_{46}Al_7$ metallic glass. The initial atomic structure can be visualized in Figure 1.

The next steps involve defining atomic interactions using an EAM potential suitable for Al-Cu-Zr systems, followed by energy minimization using the conjugate gradient (CG) method to stabilize the initial structure. The system is then heated from 300 K to 2100 K, ensuring it reaches a molten state. After heating, the metallic glass is equilibrated at 2100 K to allow atomic rearrangement. Subsequently, the system is cooled back to 300 K to form an amorphous structure. A final equilibration is conducted at room temperature to complete the simulation. The cooling rate corresponds to approximately 10^{12} K/s.

It is important to note that all key parameters and conditions—such as melting temperature, cooling rate, and simulation methodology—are based on materials science literature and a referenced research article [1].

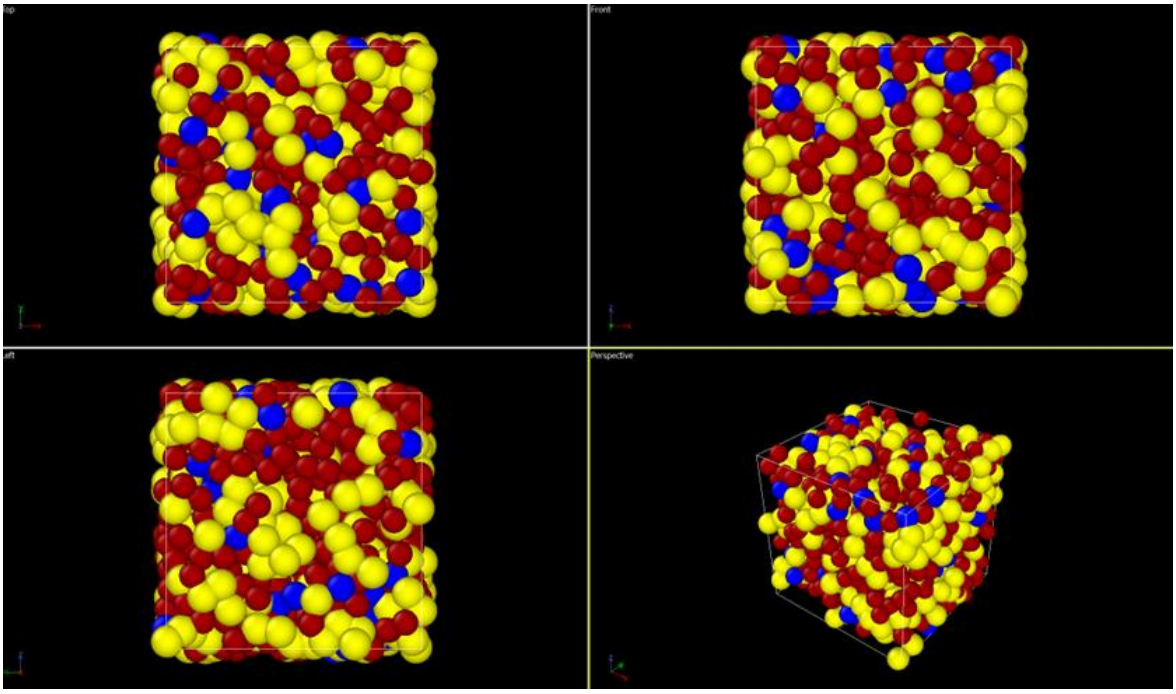

Fig. 1. Initial configuration of the simulated box viewed from multiple perspectives. Red atoms represent Cu, blue atoms represent Al, and yellow atoms represent Zr.

2. Results and Discussion

2.1. Radial Distribution Function Analysis

Based on LAMMPS documentation, By default the radial distribution function (RDF) is computed out to the maximum force cutoff defined by the `pair_style` command. If the cutoff keyword is used, then the RDF is computed accurately out to the Rcut $>$ 0.0 distance specified.

In this project, the radial distribution function was measured using the Coordination Analysis modifier in OVITO. Alternatively, it can also be calculated directly in LAMMPS using the compute `rdf` command. Figure 2 presents the changes in the radial distribution function of the simulated metallic glass at every 300 K interval. Increasing the time steps during the equilibration phase at both 2100 K and 300 K does not alter the pattern of the RDF output and has a full similarity with RDF of project article. This indicates that the simulated atomic metallic glass remains in equilibrium after the defined time steps have been completed. It shows the evolution of the RDF at intervals of 300 K. The RDF remains consistent throughout the equilibration stages at both 2100 K and 300 K, even when additional timesteps are included. This consistency indicates that the system has successfully reached equilibrium under the specified simulation conditions.

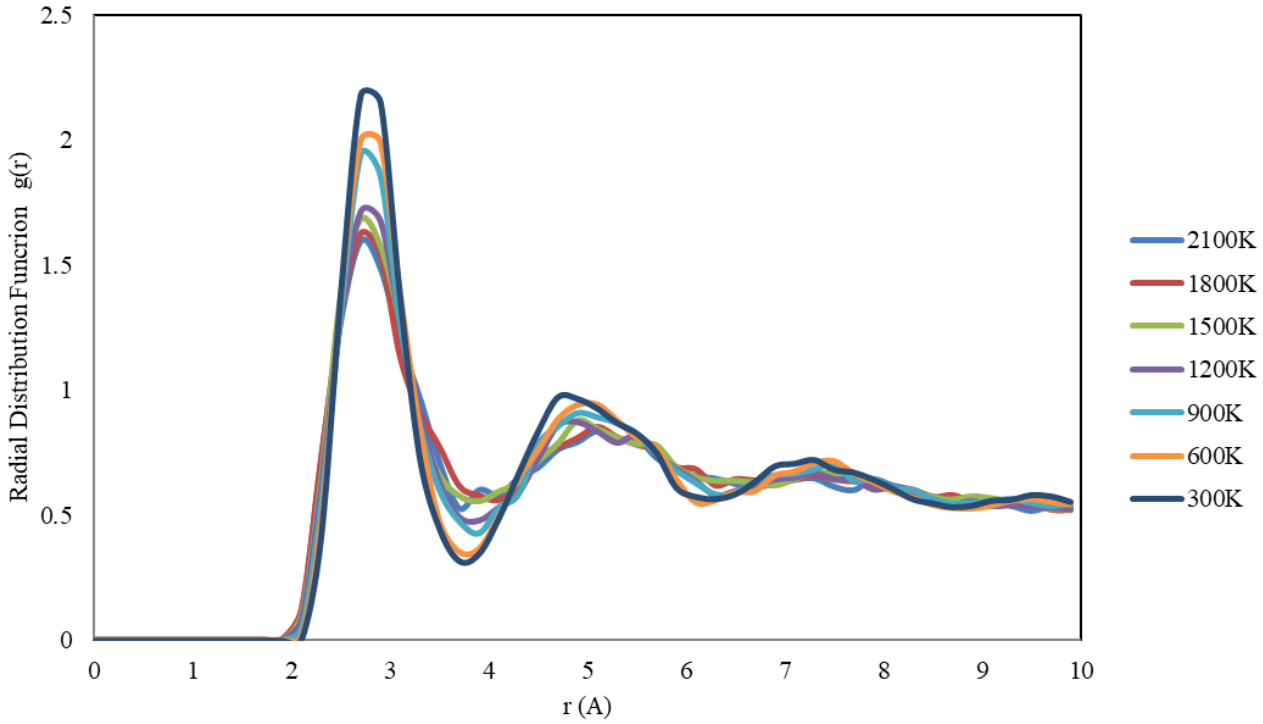

Fig. 2. Radial distribution function of the simulated $Zr_{47}Cu_{46}Al_7$ metallic glass at 300 K intervals, ranging from 2100 K to 300 K.

2.2. Voronoi Tessellation

In this section, the number of icosahedral clusters formed within the simulation box is computed using Voronoi analysis in OVITO. The numerical variation of icosahedral cluster populations at different temperatures is illustrated in Figure 3.

As in the RDF analysis, the results were obtained after confirming equilibrium at both 2100 K and 300 K. Extending the simulation time during the equilibration phase does not significantly alter the number of icosahedral clusters, indicating that the simulation duration is sufficient for the system to reach equilibrium.

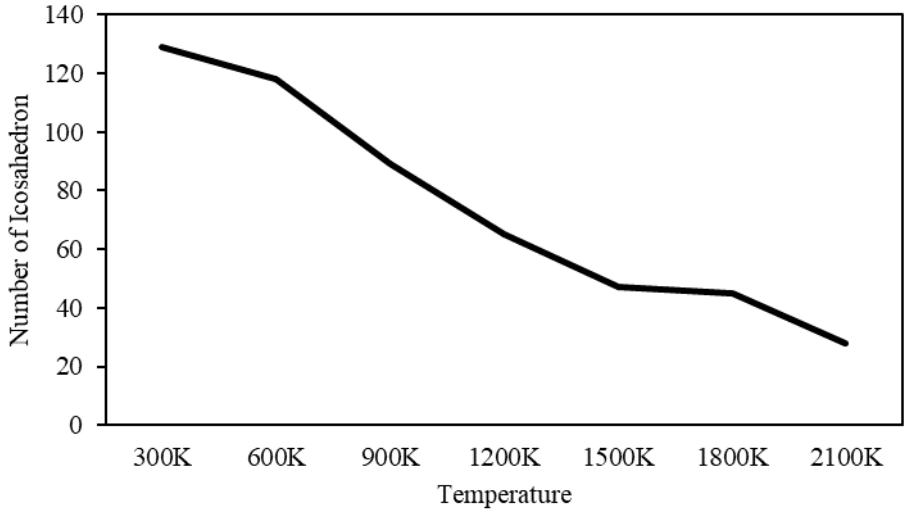

Fig. 3. Number of icosahedral clusters at different temperatures.

Figure 4 shows the output of the Voronoi analysis at 300 K, highlighting the structural evolution of the metallic glass. No significant differences are observed between the Voronoi structures at 2100 K and 300 K, further confirming that the system has equilibrated at both temperatures.

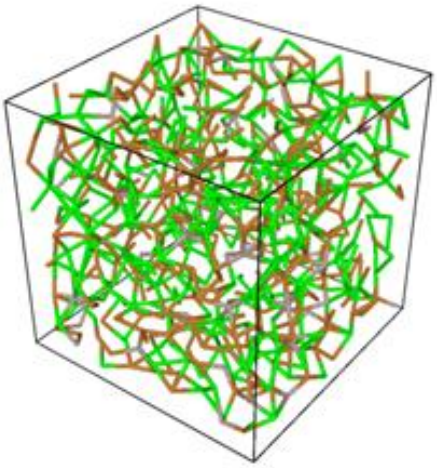

Fig. 4. Voronoi analysis of the simulated $Zr_{47}Cu_{46}Al_7$ metallic glass at 300 K.

2.3. Atomic Radius

In this section, a method for estimating the atomic radii of Al, Cu, and Zr atoms in the simulated metallic glass is presented. The total volume occupied by the atomic structure was computed using the Construct Surface Mesh modifier in OVITO. By combining the calculated volume with the known atomic percentages of the $Zr_{47}Cu_{46}Al_7$ composition, the approximate atomic radii were determined. The resulting values are approximately 1.40 Å for Al, 1.26 Å for Cu, and 1.57 Å for Zr. Minor discrepancies in these values are expected due to potential computational errors in volume estimation performed by the OVITO software.

Reference

[1] Y. Q. Cheng, E. Ma, and H. W. Sheng, "Atomic level structure in multicomponent bulk metallic glass," *Phys Rev Lett*, vol. 102, no. 24, p. 245501, 2009.