Evaluation of Pair Potentials at Different Temperatures for Molecular Dynamics Simulation of Sintering

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Description of Sintering

Sintering is a material process using finely divided grains of metal.

Powder can be compacted into a mold and heated to form a solid object.

Benefits of this process

• Low processing time → near net shape forming
• Low waste
• Energy efficient → does not need to reach melting point to fuse
Molecular Dynamics

- High resolution method of modeling
- Calculates force between a single atom and its neighbors
- Computationally intensive
- Forces calculated via a potential type

Sample from current efforts:
- Blue - copper, Red - Aluminum
- ~13,000 atoms
- Run at 900K below the melting point
- Total run time represents 64 nano-seconds
**Simulation**

- Simulation is done on blocks of metal for simplicity
- Run a range of temperatures based off melting point
- ~32500 atoms
  - 14250 Aluminum
  - 18250 Copper

**Computer Cluster**

- Cluster is made of 7 Raspberry Pis each with 4 cores
- Longest simulation took 15 hours
- Shortest Simulation to 4 hours
- While simulation time is 431 nano-seconds
Diffusion Coefficient

- Diffusion Coefficient is a mass transfer quantity to track the motion of atoms in the system
- LAMMPS has two means of calculating diffusion: mean squared displacement and velocity auto-correlation function
- Used mean squared displacement because of the excessive noise and fluctuation in the other method

Impact of Work

- Diffusion Coefficient can be used directly in other models as an input
- Multi-element metals have not been well studied in MD
Lennard-Jones (LJ) Potential

\[ E = 4\varepsilon \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right) \]

\[ E = 4\varepsilon \left( \left( \frac{\sigma}{r} \right)^{9} - \left( \frac{\sigma}{r} \right)^{6} \right) \]

\( \varepsilon \): depth of energy well
\( \sigma \): zero cross distance
\( r \): interaction distance

12/6

9/6

- Very low computational cost
- Needs very little input data
- Frequently used to model fluids
- Inputs can be modified for theoretical conditions
- However, doesn’t reflect reality sometimes

*While values are given for pure elements no such information exists for compounds or alloys. Instead, an average value must be taken and used.*
EAM/MEAM potential

EAM

\[ E_i = F_\alpha \left( \sum_{j \neq l} \rho_\beta (r_{ij}) \right) + \frac{1}{2} \sum_{j \neq l} \phi_{\alpha\beta} (r_{ij}) \]

MEAM

\[ E = \sum_i \left\{ F_i \rho_i + \frac{1}{2} \sum_{i \neq j} \phi_{ij} r_{ij} \right\} \]

- Works well for a variety of materials
- EAM and MEAM need experimental data to function
- EAM has many permutations to accommodate its shortcomings
- Difference between the two has to do with how the embedding functions is applied

F: Embedding Energy
\( \rho \): Electron Density
\( \phi \): pair potential
interaction
\( r \): interaction radius

Potentials come from NIST: https://www.ctcms.nist.gov/potentials/
Simulation Operations

Temperature range for sitting is between 0.7 and full value of the melting point.

- Used the lower melting aluminum as basis of range.

- Cumulative run time for each potential tested:
  - LJ9/6: 175 hours × 28 CPU cores
  - LJ12/6: 110 hours × 28 CPU cores
  - EAM: 200 hours × 28 CPU cores
  - MEAM: 340 hours × 28 CPU cores

- In total: 175 Simulations
- 23,100 CPU hours

Number of Trials per Temperature Point

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<th>Temperature</th>
<th>0.70$T_m$</th>
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</table>

$T_m$: melting temperature
LJ Diffusion Results

- Results clearly show erratic data
- And a look at the max temperature diffusion shows a lack of atomic movement
- Qualitatively no diffusion between the materials has occurred
*Not suitable for use in this temperature range*

**Models just below the Melting Point**

![LJ 9/6](image1.png)  ![LJ 12/6](image2.png)
EAM Diffusion Results

- Diffusion trends upward with temperature
- Shows a sharp change right near melting
- Clear diffusion and rearrangement of material to a lower energy state
- Of the two EAM is less computationally intensive, requiring a shorter run time
- Either can be used, but EAM will require less fitting
Concluding Remarks

• Molecular Dynamics provides a powerful means of gathering material properties
• Raspberry Pi cluster provides a cost-effective means of performing MD simulations
• Among the tested potentials, only EAM provides realistic response
• More work is required for multi-element systems — a Research Opportunity to publish peer-reviewed research papers
• Future efforts will be directed at fitting and closer model agreement
Acknowledgement

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Thank you for viewing our presentation. Any questions?