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Final Report

DOE AWARD NO. DE-SC0022999 PI MARKUS BUEHLER

a. **DOE Award # and name of the recipient (Institution).**

DOE Award #: DE-SC0022999

Name of Recipient Institution: Massachusetts Institute of Technology

b. Project title and name of the PI (and co-PIs, if any).

Project title: Machine learning assisted prediction of tungsten heavy alloy plasma facing component performance for fusion energy applications

Name of PI: Markus Buehler

c. Date of the report and research period covered by the report.

Date of report: 05/05/2024

Period covered by report: 09/01/2022—08/31/2023

d. A brief description of accomplishments from the DOE award. Use an appropriate format to indicate progress.

Please see report beginning on next page.

Machine learning assisted prediction of tungsten heavy alloy plasma facing component performance for fusion energy applications

Summary: Tungsten and tungsten heavy alloys (WHAs), known for their remarkably high hardness, durability, and corrosion resistance[1,2], play a critical role in the thriving development of nuclear fusion reactors in recent years[3]. However, the exploration in tungsten alloys for the nuclear-related applications has been limited by the difficulty of manufacturing and the complexity of experiments to reproduce the environment of nuclear reaction. Therefore, this project aims to utilize nanoscale simulation methods such as density functional theory (DFT)[4] and molecular dynamics (MD)[5] with the help of machine learning techniques to not only understand the mechanisms of tungsten alloys but also allow us to computationally predict their mechanical behaviors under extreme environments.

One critical problem of the application of WHAs in nuclear reactors is the surface melting. In the current design of the SPARC reactor, the WHA, W97Ni2.1Fe0.9 or W97NiFe, is chosen to be the first wall components to confine the plasma where the particles are fiercely moving and colliding into each other to create nuclear fusion reaction. This process will generate extremely high heat flux onto these WHA tiles, leaving high surface temperature that could possibly melt the surface of the WHA tiles, As illustrated in Fig. 1(a). a laser experiment previously done illustrates that a rough surface damage would be made after the surface melting where the matrix area mainly composed of nickel and iron as shown in Fig. 1(b), will first melt and then leave vacancies between these tungsten grains. Unfortunately, these kinds of roughness on the first-wall components could be deadly to the plasma inside a Tokmak reactor because the heat that is supposed to dissipate at a designed ratio through the tiles may in turn be excessively absorbed and accumulated on any uneven area of the surface, which will eventually make the whole nuclear reaction fail. In this project, we will introduce a machine learning potential, Allegro[6], based on DFT calculation and then build a MD model for W-Ni-Fe alloys.

Objectives

The main goal of this project is to investigate and predict the mechanical performance of WHA under high temperatures. Since our targeted W97 heavy alloys and its other W-Ni-Fe family have rarely been studied, we are starting with quantum-level simulation methods, using Vienna Ab initio Simulation Package (VASP)[7], to first computationally realize their fundamental mechanisms as illustrated in Fig. 1(c). And since DFT simulations are so expensive that it is impractical to use them to model physical phenomenon at the microscales. We will then apply machine learning techniques to train our own potential specializing for W-Ni-Fe interactions, bridging the quantum-level calculation to a nanoscale simulation method such as MD simulation to keep both the efficiency and accuracy. We will then use Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)[8] to study the mechanical behaviors of W97 alloys at high temperatures to show the reaction of W97 alloys subject to the extreme heat flux inside a SPARC reactor.

Results

Allegro Machine Learning Potential Training and MD Simulation Results

As shown in Fig. 2(a), the training history of Allegro potential for W-Ni-Fe alloys shows great convergency on both loss and accuracy, which implies that the Allegro model can capture the physical meanings in the DFT dataset. Then, as shown in Fig. 2(b), with NVT ensemble, our MD model can simulate the sample of W97 alloy in Fig. 1(b) to generate a complete temperature profile from 300K to 4000K. The result shows great credibility as the heating curve goes up smoothly. The movie of the heating simulation can be found via this link: https://shorturl.at/FNOU3.

Method

Density Functional Theory Simulation

The DFT ab-initio simulation is carried out by VASP and its tungsten, nickel, and iron pseudopotentials. There are totally 131 simulation cases collected from DFT calculation. One single case in the dataset is shown as below. To train a machine learning potential such as Allegro with DFT calculation results, it usually takes a) the number of atoms, b) the lattice geometry, c) boundary conditions, d) atom species, positions and forces, and finally e) system energy, following the same order as in the text box below.

```
30
Lattice=" 8.952538 0.0 0.0 0.0 8.952538 0.0 0.0 0.0 6.3304" PBC="T T T"
Properties=species:S:1:pos:R:3:forces:R:3 energy=-282.29977513 "
W 0.00899 0.00739 6.31906 -0.247885 -0.550854 0.06909
W 2.23134 0.00772 1.59352 -0.329689 -1.340804 -0.333477
…
Ni 4.44178 4.49672 3.12992 -0.814724 1.238037 -0.036772
Ni 6.22915 4.501 1.33361 1.16247 1.065651 -0.401559
…
Fe 4.4747 6.22948 4.9893 -0.135258 0.438462 0.312901
Fe 4.50377 7.85063 3.1513 0.199664 -5.656032 -0.1121
```

Allegro Machine Learning Potential

The model structure is shown in Fig. 3(a, b). The idea of the Allegro model is to consider all the pairs would only have the contribution only from the neighbor atoms within a strictly local environment. The model adopts Euclidean representation for atom and pair information and then use tensor product to combine and project them onto a vector space, which can then keep as much the physical and geometrical information as much as possible.

Molecular Dynamics Simulation

The MD simulation is carried out by LAMMPS compiled with pair_allegro: https://github.com/mir-group/pair_allegro. We simulate a thin plate, with two half-size grains and matrix area in the middle as previously shown in Fig. 1(b), with full periodic boundaries and NVT ensemble to mimic the physical behaviors of the W97 alloy surface near the grain-matrix boundaries. In the movie mentioned earlier we can see how the nickel and iron particles in matrix area are agitated and then turned into liquid phase while the rest of the tungsten grains remain relatively stable.

Discussion and Conclusion

Over the past few decades, although tungsten and its derivatives are widely applied in many fields, there is not much progress on its application on nuclear engineering field because it is unrealistic to investigate their performance by nuclear infusion experiment. Thanks to the Allegro potential, we now have the MD simulation model first ever built for W-Ni-Fe alloys. With this model, we can efficiently probe the mechanical behaviors of different WHA samples. In addition, the scalability is also guaranteed since the Allegro potential by its nature is a strictly locally computed force potential, which means we can tune up the length scale of simulation model to include more complicated geometries if required. However, one limitation of the current approach is that the mechanical properties involving stress components may not be correctly reported as this method is still under development, which will be addressed in the next phase of this project as the future work. To conclude, this DFT-based MD model can provide promising simulation result for nuclear engineers to understand the underlying mechanisms of surface melting on WHA tiles.

References

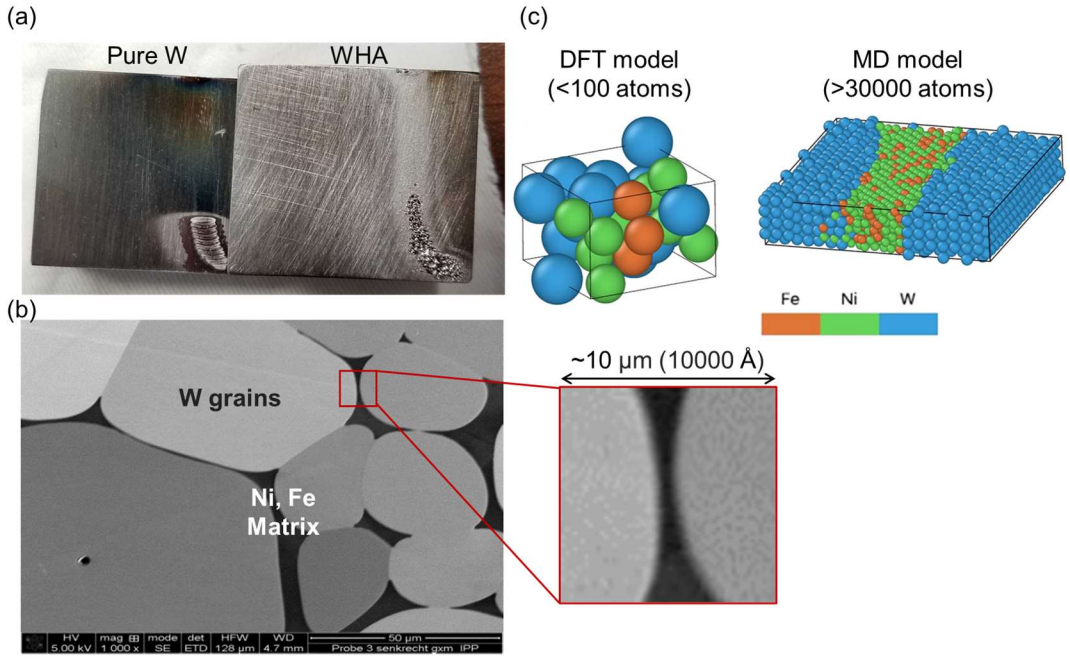

Figure 1. (a) The pictures of samples, pure tungsten and W97 tungsten heavy alloy, after the laser beam experiment. (b) An SEM image of tungsten heavy alloy that shows grain and matrix microstructure in W97 alloy and the sample (in red square) for our (c) MD simulation model. The DFT model for is shown in (c)

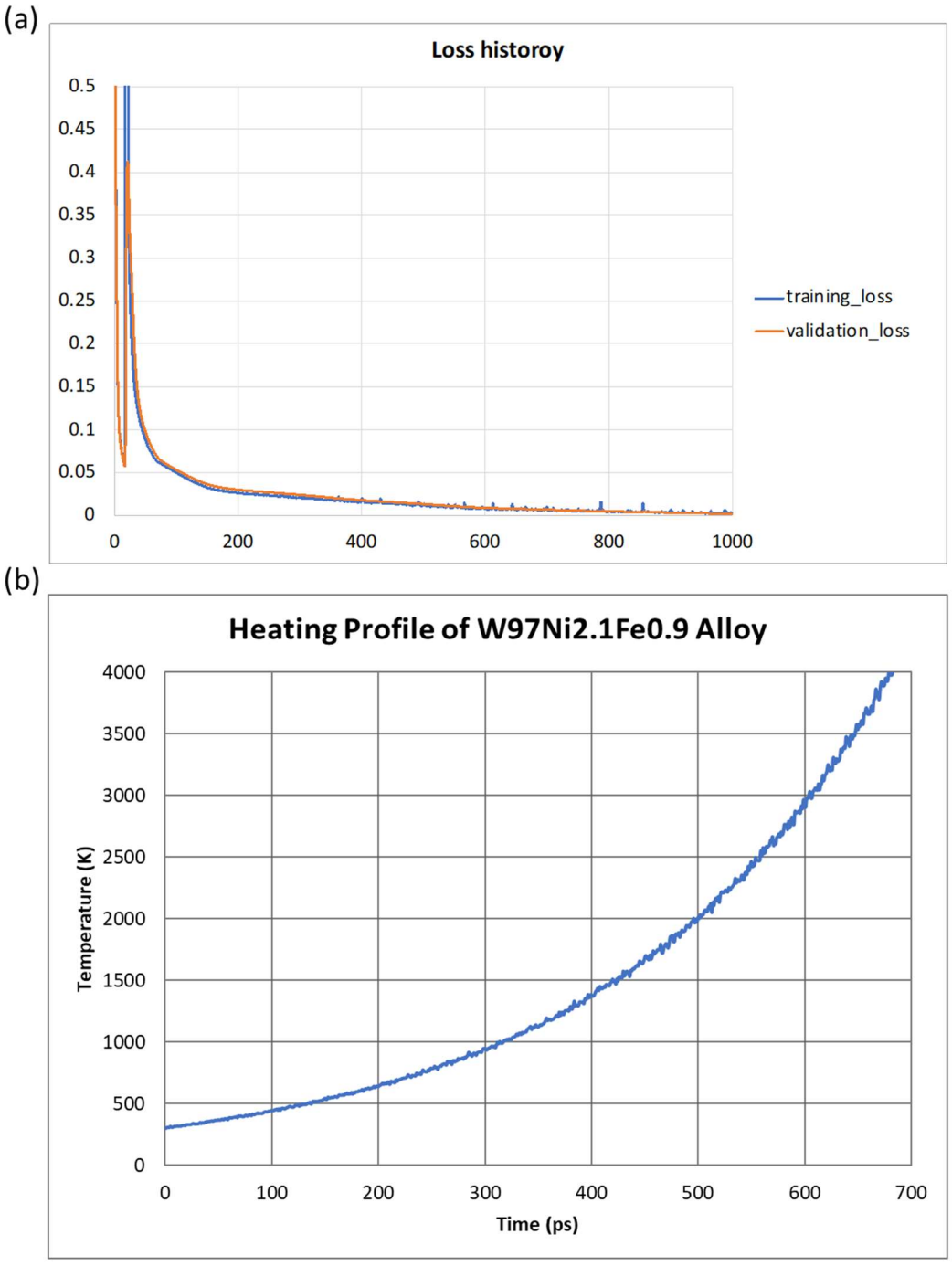

Figure 2. (a) the training history of Allegro potential against DFT dataset and (b) the heat profile of the W97 sample simulated by LAMMPS and pair Allegro.

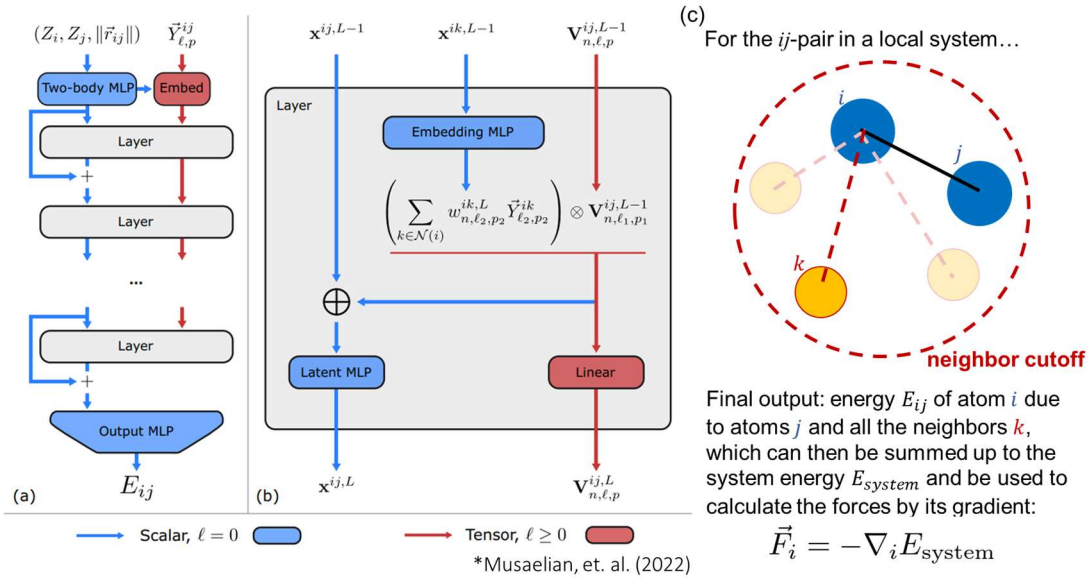

Figure 3. (a, b) The allegro model structure (adapted from the original paper[8]) and (c) the illustration of the strictly local environment of Allegro potential.

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e. A list of papers (mark as published, in press, or submitted) in which DOE support is acknowledged. Attach copies of manuscripts that have been prepared but not yet submitted for publication.

A paper is in preparation, but has not yet been published.

f. A comprehensive list of people working on the project – graduate students, postdocs, visitors, technicians, etc. Indicate for each the percentage of support obtained from the grant.

- Yu-Chuan Hsu, Graduate Research Assistant:
  - 100% support, 09/01/23-07/31/23;
  - 80% support, 08/01/22-08/31/23
- Wei Lu, Graduate Research Assistant: 100% support, 06/01/23-06/30/23
- Talia Khan, Graduate Research Assistant: 1.79% support, 06/01/23-08/31/23

g. **Estimate of the unexpended funds at the end of the final budget period; if funds exceed 10% of the annual budget, provide a detailed explanation.**

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