鉄加工におけるダイヤモンド工具の摩耗： 機械学習分子動力学アプローチ
Diamond Tool Wear in Iron Machining: A Machine Learning Molecular Dynamics Approach

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1. Objectives

Ferrous metals, known for their mechanical strength, are widely used in engineering and often require ultra-precision machining. While diamond tools are ideal for such tasks, they wear rapidly when cutting iron—a material considered non-diamond-turnable. This rapid degradation is linked to unclear thermo-chemical reactions at the Fe-C interface. Our research aims to clarify these reactions using machine-learning interatomic potentials.

2. Methodologies and Workflow

We start with Density Functional Theory (DFT) calculations using the STATE-senri code[1] to generate accurate atomic interaction data. This serves as the training set for developing a machine-learned interatomic potential using Allegro[2], a graph neural network framework that achieves DFT-level accuracy with lower computational cost. The trained potential is then used in molecular dynamics simulations with LAMMPS[3] to study material behavior at larger scales. Finally, Python and OVITO are used for data analysis and visualization. This workflow is iterative, allowing MD results to refine the potential through retraining.

3. Simulation Model

Large-scale cutting simulations involving over 8,000 atoms were conducted using a timestep of 1 fs and cutting durations on the nanosecond scale. Each part (tool/workpiece) has three layers: a fixed boundary layer, an NVT layer for temperature control, and an NVE (Newtonian) layer where atoms move freely; the system is periodic in x and y directions, with the tool moving toward the lower-left, as in Figure 1. To save time and ensure continuity, metal chips are removed and fresh layers added. Wear atoms are identified using a 1.9 Å cut-off; any atom or cluster disconnected from the main body is counted as wear.

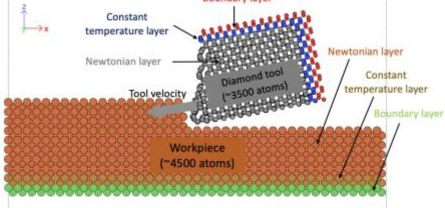

Figure 1. Simulation model

4. Results and Discussion

The ML-MD model was trained on a dataset comprising approximately 6,000 structural configurations, requiring less than one day of computational time. The resulting model achieved high accuracy, with root-mean-square errors (RMSE) of ~130 meV/Å for forces and ~4 meV/atom for energies.

Figure 2 shows the number of wear atoms during cutting time for two cases of a same tool, which has two facets, one is (100) and another is (011), the role of clearance face and rake face is switched by rotating the tool, cutting velocity and temperature of nvt layer is 50 m/s and 1073 K, respectively. For a given surface facet, clearance face wears faster than the rake face, which directly affects the accuracy of cutting, increases roughness of machined surface and requires for the tool replacement.

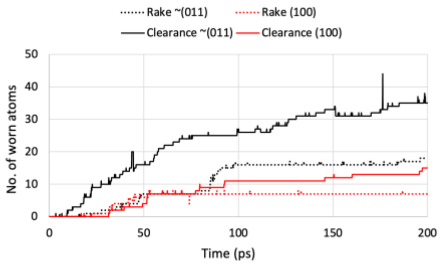

Figure 2. Dependence of wear on rake-clearance face

The temperature dependence of tool wear is shown as in Figure 3. Three different temperatures 300K, 673K, 1073K are applied to the nvt layers of a tool that have clearance face (100), rake face (011), cutting velocity is 10m/s. It could be seen that wear increases as the temperature rises, which suggests that maintaining a lower cutting temperature can effectively reduce the wear rate of the tool.

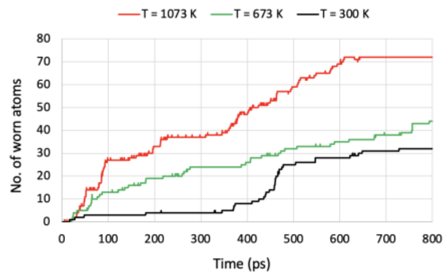

Figure 3. Dependence of wear on temperature of cutting

In practice, the (100) and (110) surfaces of diamond are commonly used to manufacture cutting tools, on the other hand, the (111) surface is difficult to fabricate and is rarely used as a cutting tool in experiments. We conducted 10 m/s velocity of cutting simulations for three (surface facet)[the direction of cutting], and the wear results are shown in the Figure 4. The (100) surface shows more resistance to wear compared to the (110) surface, but (111) surface experiences even less wear than the (100) surface. Therefore, if it can be fabricated, the (111) surface could potentially be used as a tool face.

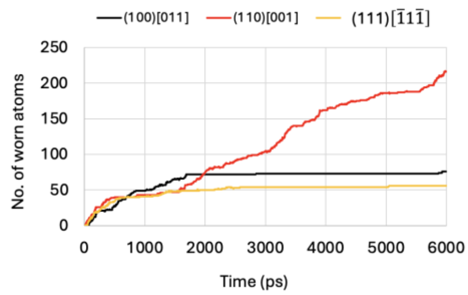

Figure 4. Dependence of wear on facet and cutting direction

During the initial nanoseconds of simulation, the calculated wear rates were 2-3 orders of magnitude higher than experimental values. It is anticipated that extended simulation durations will allow the computed wear rates to converge toward experimental observations.

References

1) Morikawa, Y., et.al, Appl. Sur. Sci 169-170, 11 (2001)

2) Musaelian, A., et.al, Nat Commun 14, 579 (2023)

3) Plimpton, S. et.al, J Comp Phys, 119, 1-19 (1995)