Neural network interatomic potentials (NNIP) for nanomechanical deformation modeling: Single-crystalline Molybdenum

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Abstract

In this work, we present the development of a ML based interatomic potential for Molybdenum (Mo) with a recently developed software called PANNA: Properties from Artificial Neural Network Architectures [4]. The elastic constants of single crystalline Mo are computed by using NNIP as well as classical EAM empirical potentials with available density functional theory (DFT) databases for Mo [2] and PANNA package to then creating the NNIP. As an application, we perform MD simulations of nanoindentation test of Mo to calculate the load-displacement (LD) curves for EAM and NNIP to describe the elastic to plastic deformation transition during loading process. Here, the dislocation nucleation and dynamics is well represented by NNIP being able to find $\langle 100 \rangle$ junction, that is important for explaining hardening mechanisms of the material.

Descriptors and training parameters

We utilize the modified Behler-Parrinello (BP) descriptors that are defined as [1].

$$G_i^{rad}[s] = \sum_{i \neq j} e^{-\eta(R_{ij}-R_s)^2} f_c(R_{ij}) \tag{1}$$

$$G_i^{Ang}[s] = 2^{1-\zeta} \sum_{j,k \neq i} [1 + cos(\theta_{ijk} - \theta_s)] e^{-\eta[(R_{ij}+R_{ik})-R_s]^2} f_c(R_{ij}) f_c(R_{ik}) \tag{2}$$

We consider the radial and angular exponents η as 10 and 6 Å^2, respectively. Also, the cut off radius (R_c) for both equations is 6.28 Å. Finally, the number of R_s (radial), R_s (Angular) and θ_s centers are 32, 8 and 16, respectively, leading to a *G-vector* of size 160.
The training was done with a learning rate of $1e^{-5}$ and targeted the total energies. The training architecture is $128:64:1$, which includes two hidden layers of 128 and 64 nodes. Here, we present preliminary results that need to be taken with care and paving the path for future research.

Training and Elastic Constants of Mo

The training is done by using an existing DFT dataset [2] which includes generally distorted crystalline Mo sub-systems and common point defects. In addition, high temperature is considered by including the liquid phase in the dataset. Fig 1a) shows the per atom energy validation (NNIP predicted energy versus DFT total energy) and noticing that the lower the energy root mean squared (RMSE), the more accurate is the evaluation as shown in b). The (RMSE) is calculated to be 29 mev/atom and the training is only done on configurational total energies, noticing that a lattice constant of 3.16 Å is obtained by both potentials.

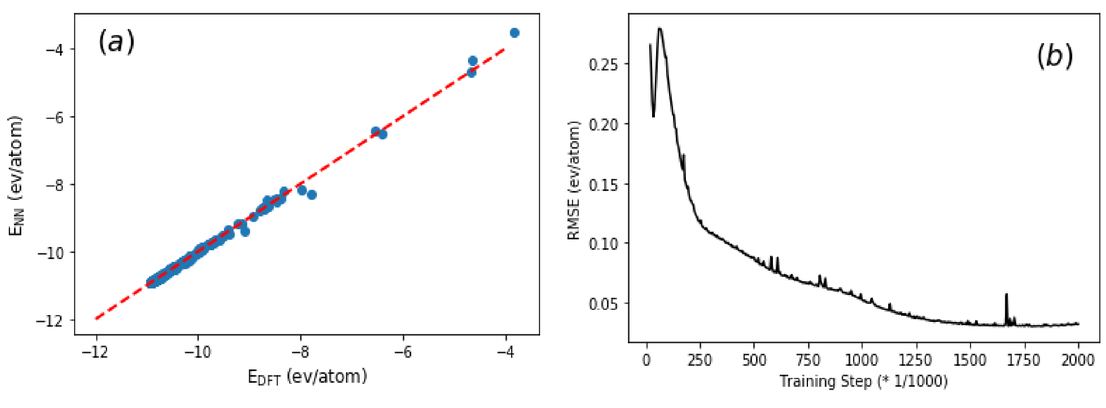

Figure 1:Energy per atom validation for the trained potential in a) and RMSE of energies in b)

The elastic constants of crystalline Mo are presented in Tab 1. Although the dataset needs to be evaluated and modified for the future work, the obtained results are fairly predicted.

Elastic Constants	EAM	PANNA	DFT	Exp.
C11 (Gpa)	464.733	423.916	468.0	464
C12 (Gpa)	161.516	123.008	155.0	159
C44 (Gpa)	108.912	125.679	100.0	109

Table 1:Elastic constants computed by different approaches.

Atomistic Dislocation nucleation modeling

Nanoindentation tests often nucleate different defects such as interstitials, screw/edge dislocations and dislocation loops in the sample. Using the above mentioned data set could be a good idea, since some defects that existed in the nanoindentation simulations are included. Figure 2 compares the load - displacement (LD) curve for EAM force field [3] and the NNIP for a system of 7000 of Mo atoms with a radius tip of 1.5nm.
As it is shown, although the curves are not exactly the same, we observe the pop-in event happening at the same depth of about 0.2 nm. Which is identified by the Hertz curve defined as: $P_H = 4/3 E_{\mathrm{H}} R^{1/2} h^{3/2}$, with an effective elastic modulus, E_{H}, of 330GPa for EAM and 325 for NIPP. LD curve for NNIP potential oscillates more than the EAM due to the lack of open surface information in the dataset.

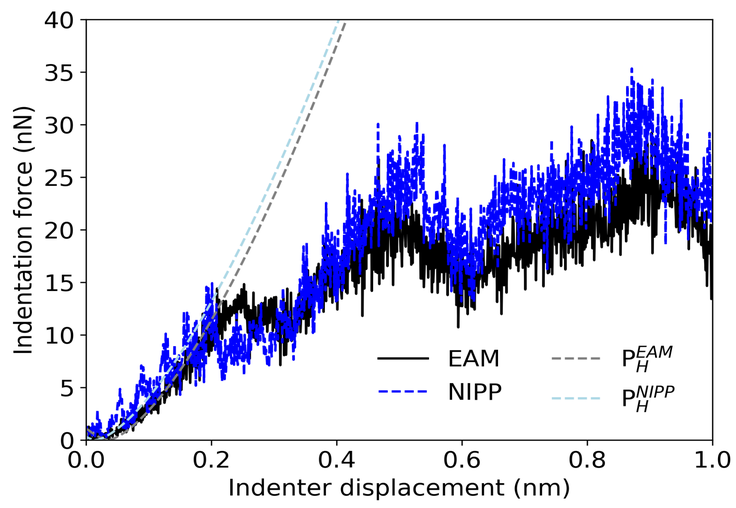

Figure 2:LD curve of the nanoindentation of crystalline Mo for the [001] orientation by EAM (solid line) and NIPP (dashed line). We fit to a Hertz curve, P_H.

Finally, Figure 3 demonstrates the dislocation nucleation at a depth = 1 nm for both EAM potential and the NNIP. It is quite interesting that NNIP can produce dislocation junctions same as EAM potential as: $1/2\langle 111 \rangle + 1/2\langle 1-1-1 \rangle = \langle 100 \rangle$; responsible of hardeness stabilization of Mo at elevated temperatures [3].

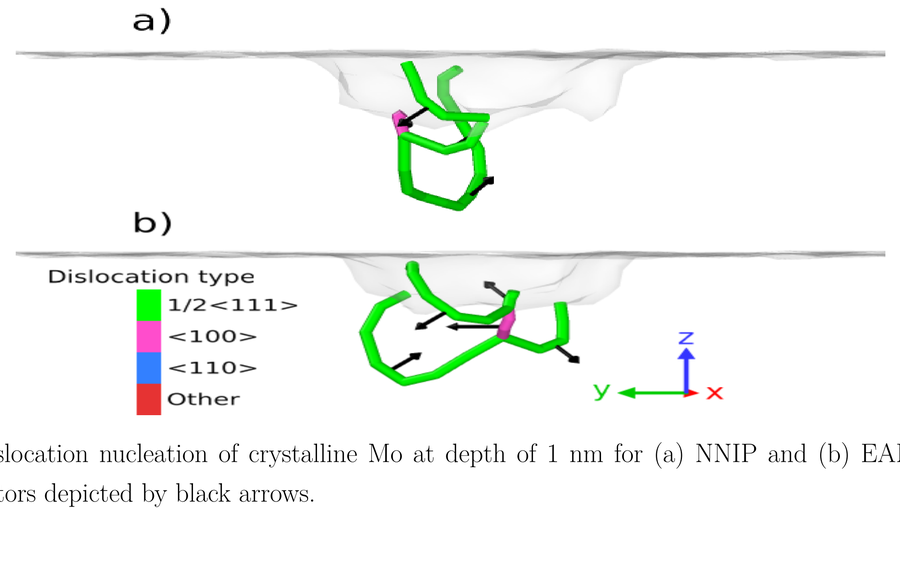

Figure 3:Dislocation nucleation of crystalline Mo at depth of 1 nm for (a) NNIP and (b) EAM potential. Burgers vectors depicted by black arrows.

Concluding remarks

We started making a benchmark for creating a machine learned based interatomic potential aiming at mechanical properties in both elastic and plastic regimes of metals and alloys. Here, PANNA framework is applied to model Mo to create a NNIP and then performed MD simulations of nanoindentation with EAM and NNIP potentials. Finally, the dislocation junctions at the maximum depth of 1 nm are well described by the new NNIP that give us the opportunity to develop further potentials for different alloys.

References

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