High-performance quadratic spectral neighbor analysis potential for Al-H binary system to investigate hydrogen embrittlement

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A wide variety of metals, including aluminum and its high-strength alloys, suffer from hydrogen embrittlement (HE). Despite that HE is an old problem and has been intensively studied since the 19th century, its mechanisms have not been comprehensively understood yet due to the difficulty in experiments of tracking hydrogen atoms with low solubility and high diffusivity. Molecular dynamics (MD) simulations based on ab-initio method and empirical interatomic potentials (EIPs) have been applied to the investigation of HE in atomic scale. However, the former is accurate but computationally demanding while the latter is fast at the sacrifice of accuracy and transferability. Since HE involves defect interaction and atom migration in large time and spatial scales, new MD simulation method is desirable for further investigation of HE. Recently, machine learning potentials (MLPs), which combine the merits of ab-initio MD and EIPs, provide us a feasible way to study HE through MD simulations with achieving larger spatial and time scales and high accuracy simultaneously.

In the present study, we constructed a MLP for Al-H binary system within the framework of quadratic spectral neighbor analysis potential (qSNAP) [1], considering its compatible accuracy and relatively light computational cost among MLPs. The root-mean-square errors (RMSE) of total energies and atomic forces of our qSNAP model, compared with DFT results, were 2.4 meV/atom and 58 meV/Å, respectively, which is comparable with the errors of well-trained neural network potential for Fe-H system [2]. Moreover, calculation results of our qSNAP model agreed well with those of DFT on various materials properties as shown in Table I and Fig. 1. In addition, a decrease in the migration barrier of H between tetrahedral and octahedral sites in bulk Al from 0.164 eV to 0.110 eV was observed with the increase of temperature from 100K to 900K. In the presentation, we will also show MD simulation results via our qSNAP model on HE.

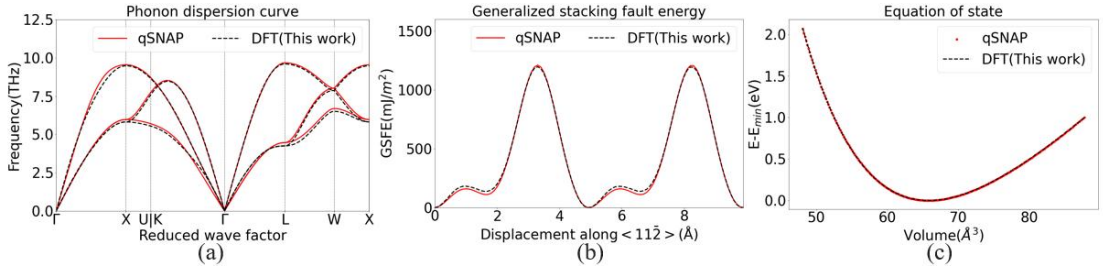

Fig. 1. Comparison of qSNAP and DFT on listed materials properties.

	a(Å)	C_{11}(GPa)	C_{12}(GPa)	C_{44}(GPa)	E_v(eV)	E_T^H(eV)	E_O^H(eV)	E_{T-O}^H(eV)
qSNAP	4.038	110.15	60.02	33.81	0.629	0.724	0.818	0.176
DFT	4.038	119.14	57.66	37.19	0.628	0.689	0.797	0.170

Table I. Properties of Al calculated by qSNAP and DFT. a: lattice constant. C_{ij}: elastic constant. E_v: vacancy formation energy, E_T^H (E_O^H): solution energy of H atom at tetrahedral (octahedral) site in bulk Al, and E_{T-O}^H: migration barrier of H between tetrahedral and octahedral site at 0K.

Reference:

[1] M, A, Wood and A. P. Thompson, J. Chem. Phys. 148, 241721 (2018).
[2] F.-S. Meng, et al., Phys. Rev. Mater. 5, 113606 (2021).