General-purpose neural network interatomic potential for the α-iron and hydrogen binary system

Osaka University
Graduate School of Engineering Science
Fan-Shun Meng , Jun-Ping Du, Shuhei Shinzato, Peijun Yu, Shigenobu Ogata

Purpose Toward atomic-scale understanding of hydrogen embrittlement

Outline Neural network interatomic potential construction and applications

Result A general-purpose neural network interatomic potential for the α-iron and hydrogen binary system was constructed based on DFT calculations. This potential can well describe α-iron, H_2 molecule and interactions of H with various defects of α-iron. The NNIP as applied to several key phenomena necessary for understanding hydrogen embrittlement, such as hydrogen charging and discharging to iron hydrogen transportation in defective α-iron, hydrogen trapping and desorption at defects and hydrogen-assisted cracking at the grain boundary.

Computing system:	Octopus
node-hour	1000 node-hour
memory used	50 GB
vector per	85 %
parallelize	2-4 nodes