# Deep neural network interatomic potentials for α-iron and α-iron–H binary system

Shihao Zhang, Fanshun Meng, Junping Du, Dan Wei, Md. Hossain Rana, Heting Liao, Yangen Li, Yujie Jia, Shuhei Shinzato and Shigenobu Ogata
Osaka University

**Purpose** Development highly efficient and transferable neural network interatomic potentials for α-iron and α-iron–H binary system.

**Outline** Train and validate the potential. Investigate hydrogen embrittlement for crack model and polycrystalline model using the potential.

**Result** The efficiency of the potential shows 40 times faster than our previous potential. Hydrogen atoms segregated at crack tip facilitate the brittle-cleavage failure of crack followed by crack growth, as well as those at GB promote the nucleation of intergranular nanovoids and leading to intergranular fracture.

| | |
|---|---|
| Computing system: | SQUID (GPU nodes) |
| node-hour | 2,000 node-hour |
| memory used | 2 TB |
| parallelize | 1 node for potential training<br>4 nodes for simulation |

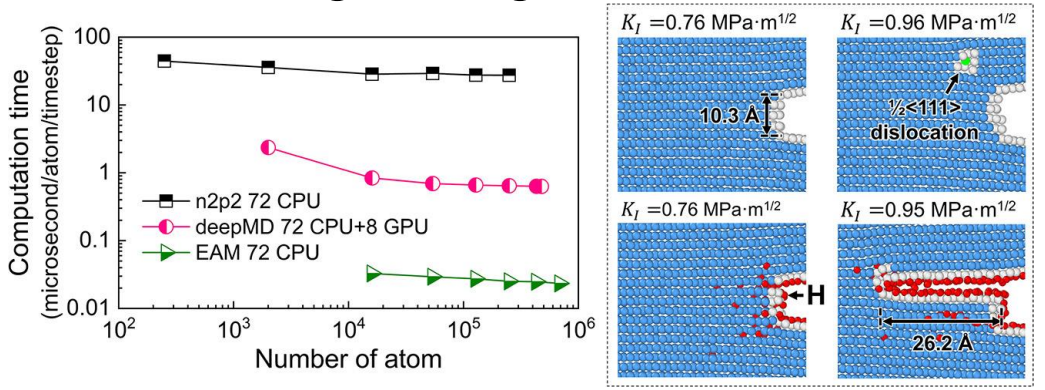


Fig. Performance of DNN potential and simulation results of crack propagation using DNN