Atomic simulation based on machine learning techniques: application to material strength problems

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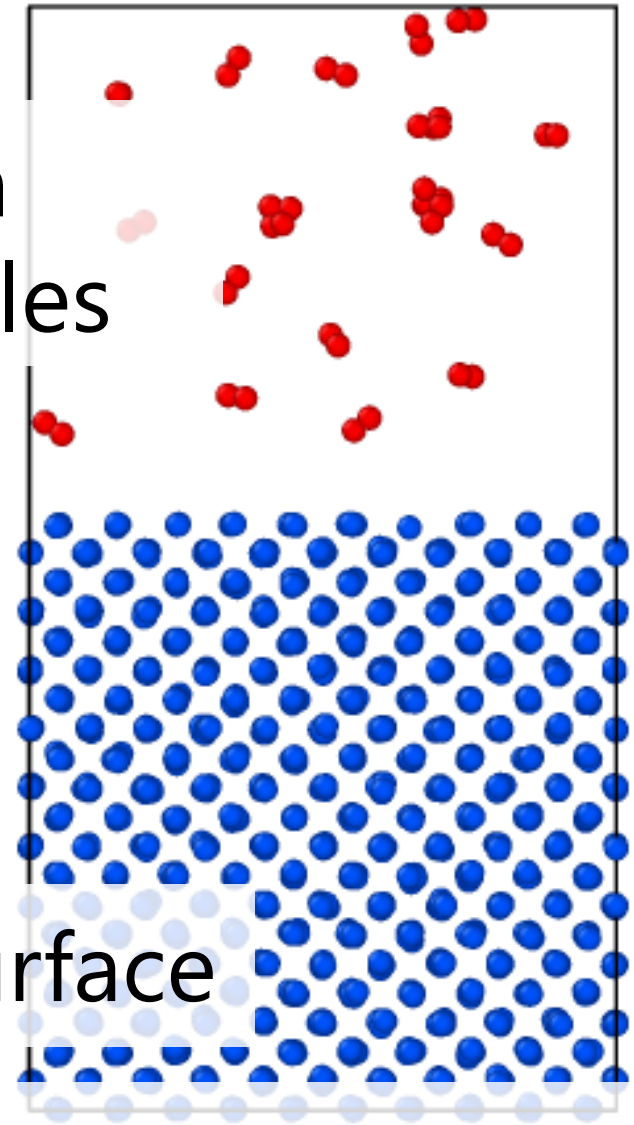
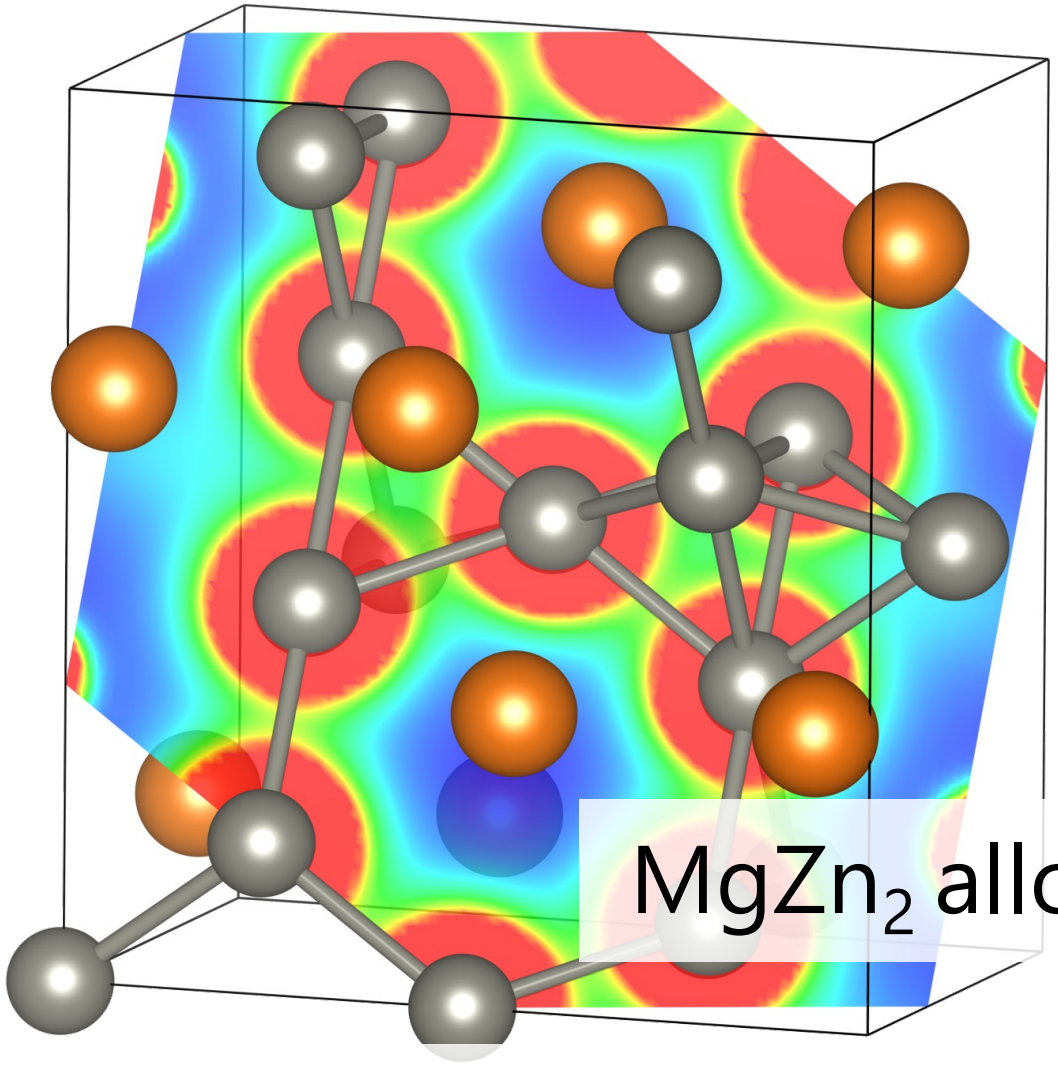
Simulations of atomic behavior

Oxygen molecules



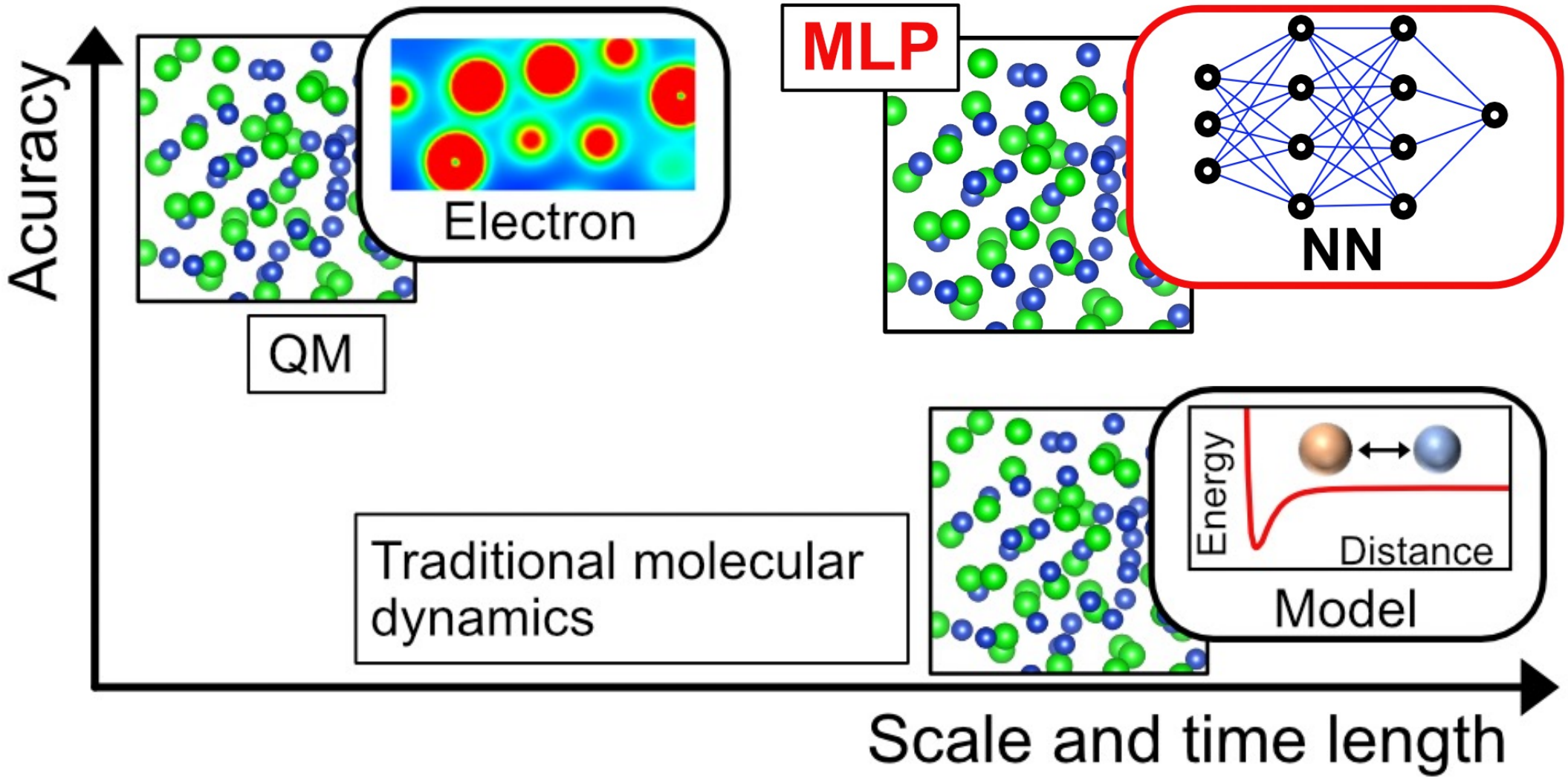
Iron surface

Molecular dynamics

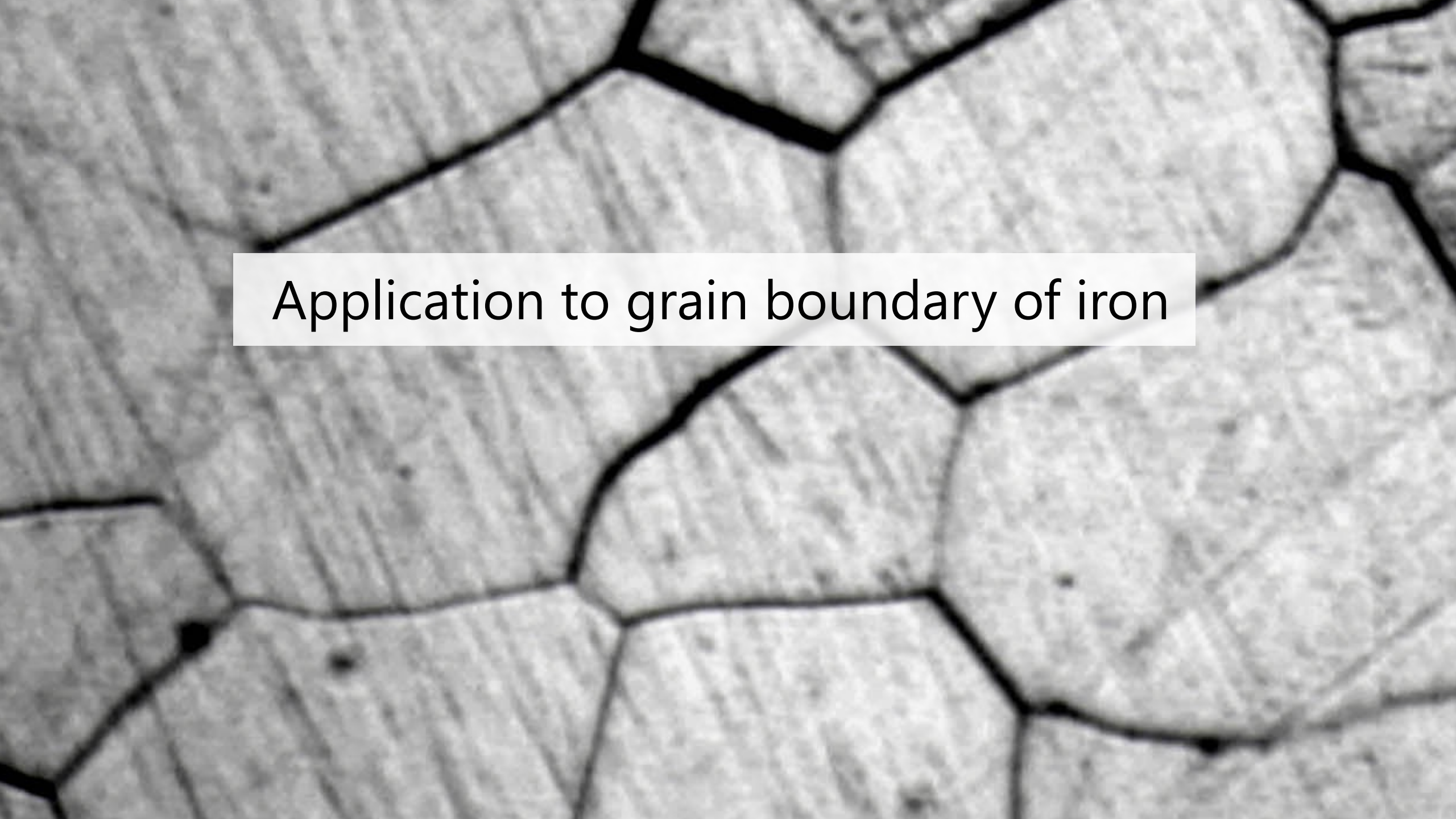


Quantum mechanics

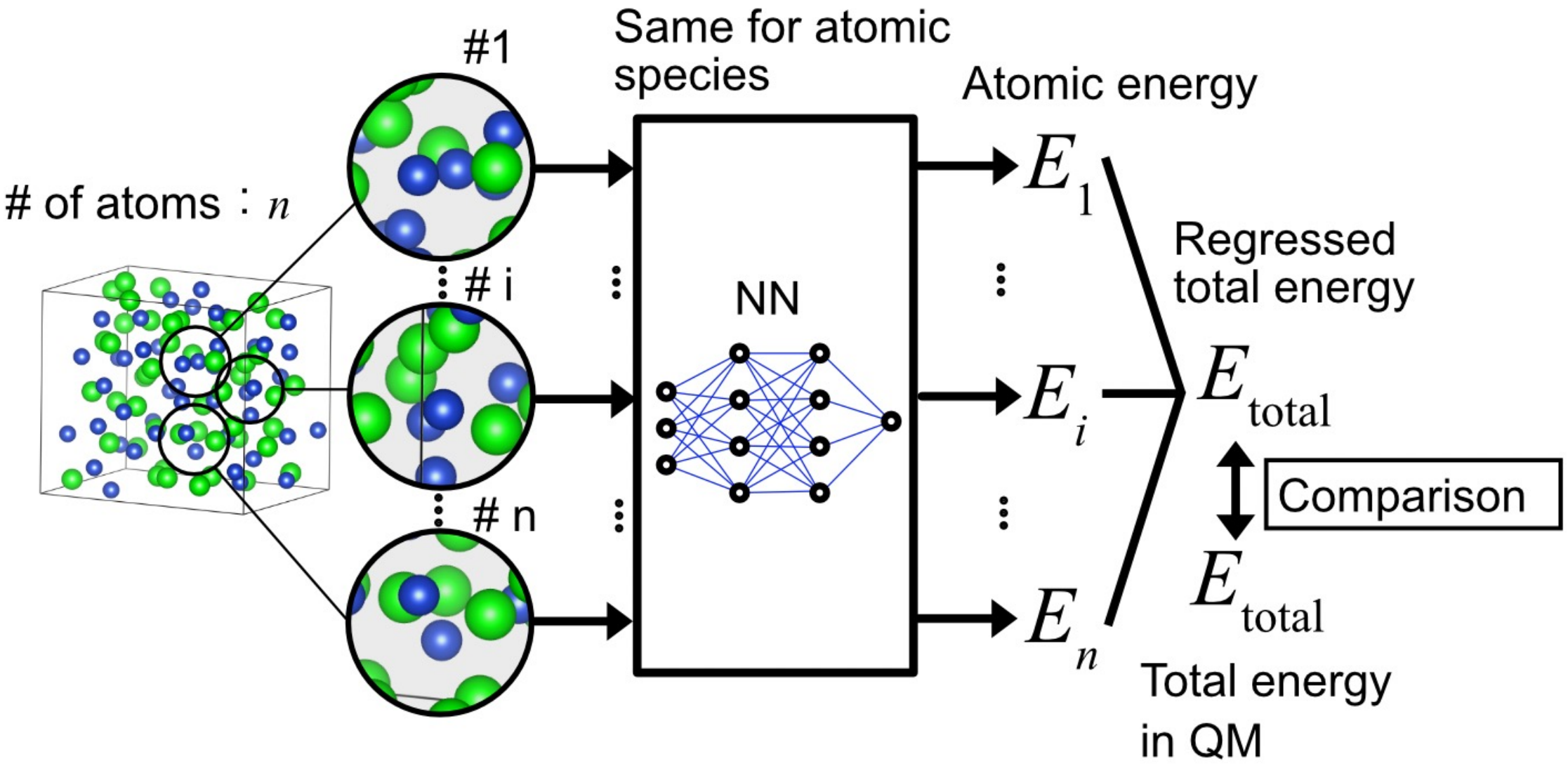
Problems in atomic simulations



Machine learning is the breakthrough.


Application to grain boundary of iron

Construction of machine learning potential

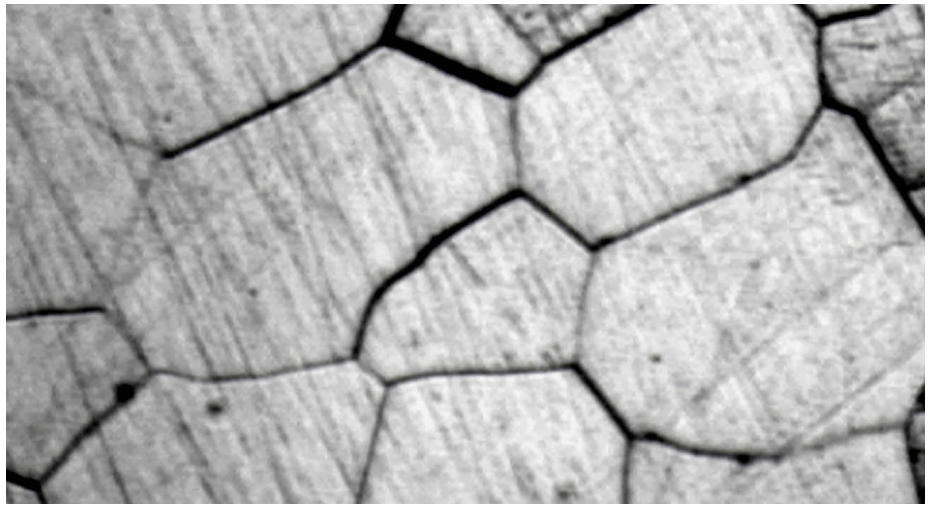


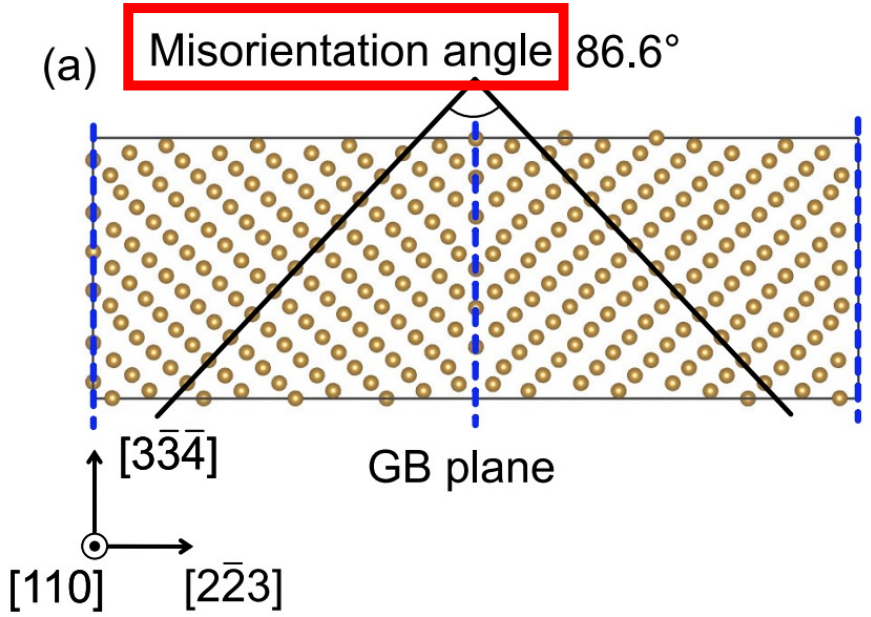
Grain boundary model

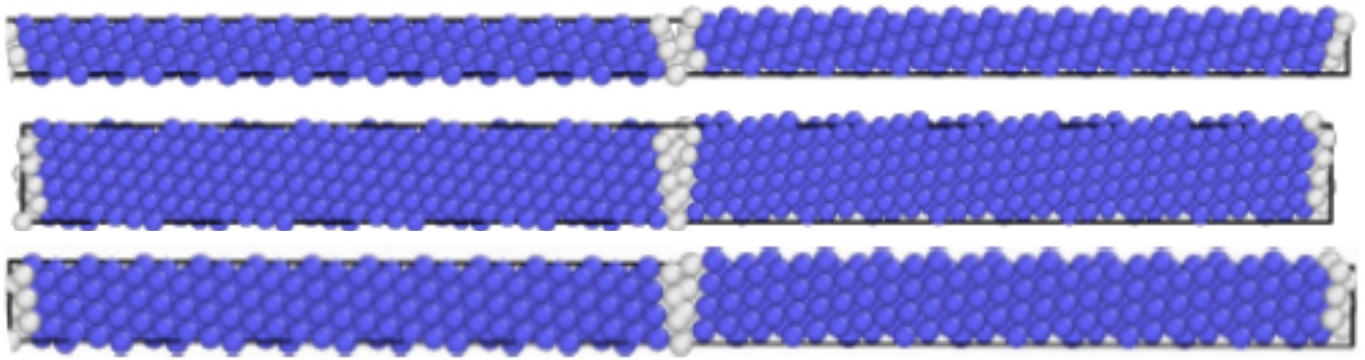
Target: calculation of grain boundary energy

$$\gamma_{\mathrm{GB}} = \frac{E_{\mathrm{GB}} - N E_{\mathrm{bulk}}}{2A}$$

represents stability of GB

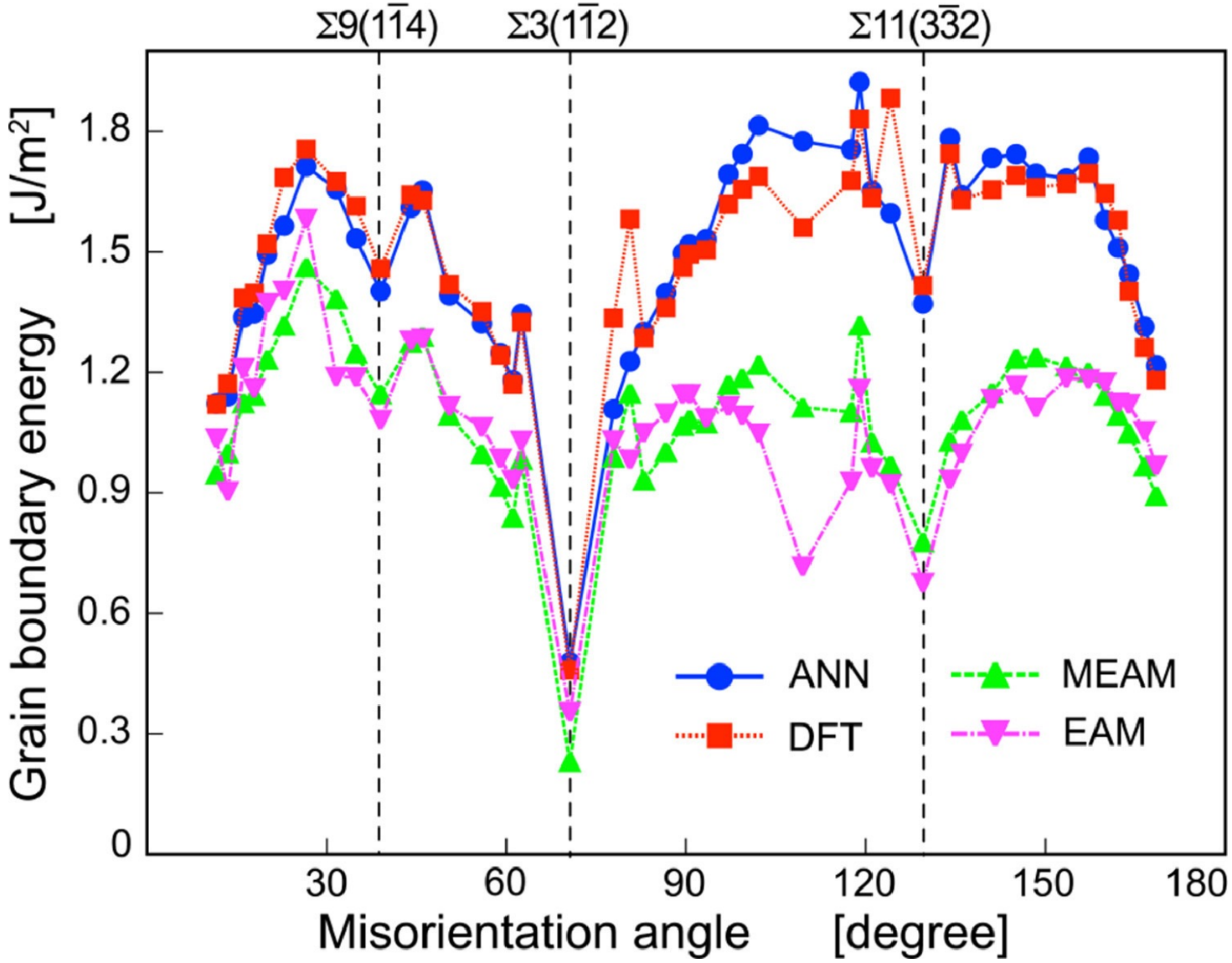






… 46 cases with different angles

Results: grain boundary energy

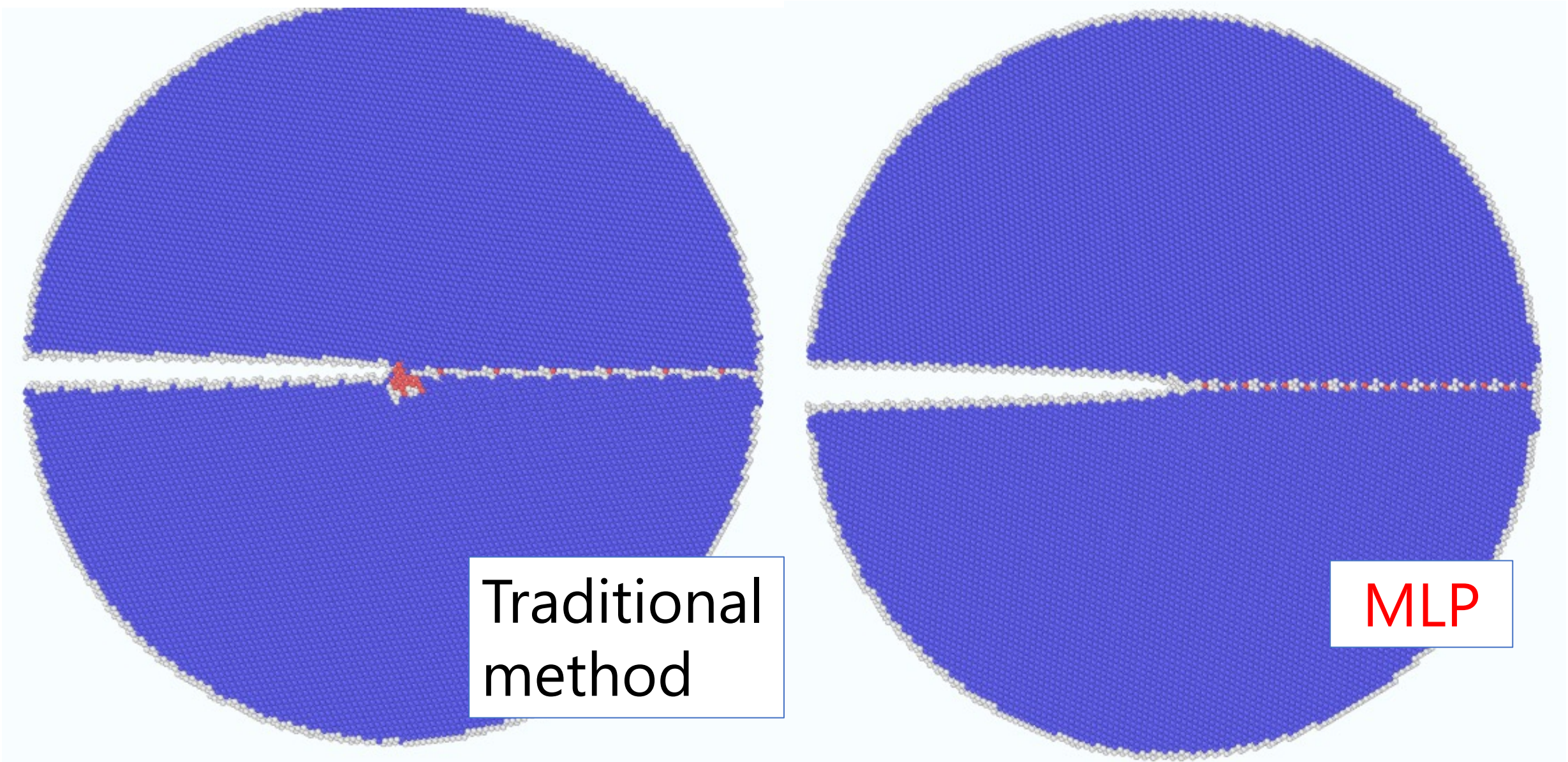


QM and MLP

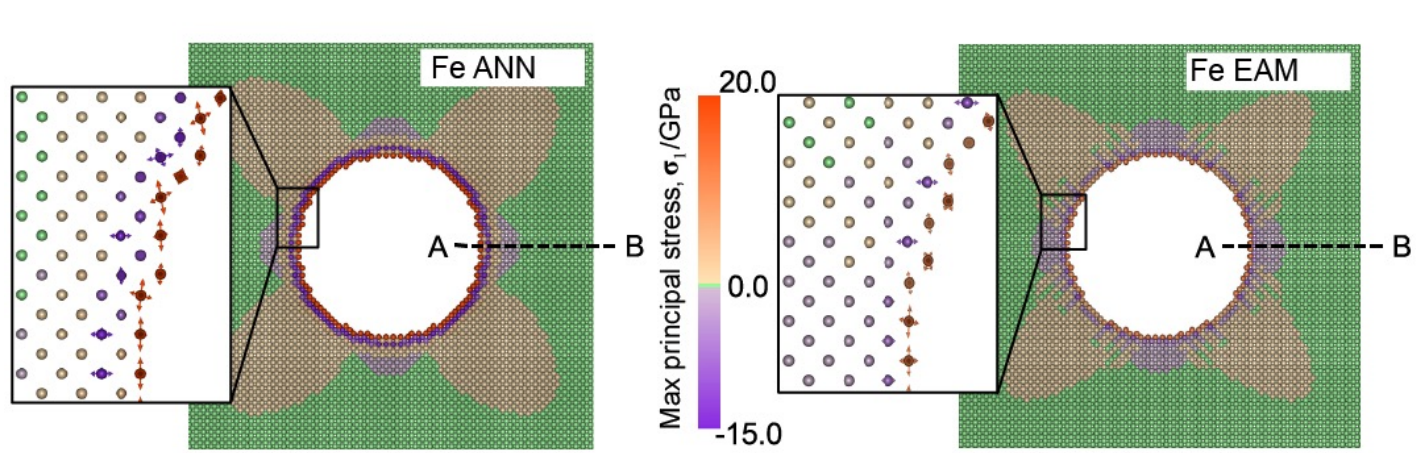
Traditional methods

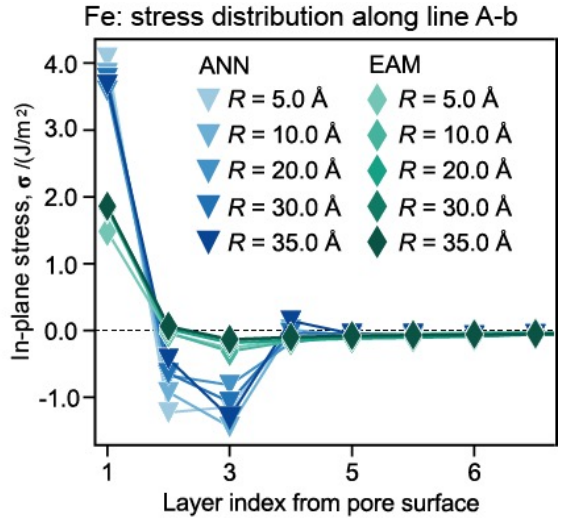
Y. Shiihara, et al.,Scripta Materialia, 207, 114268 (2022)

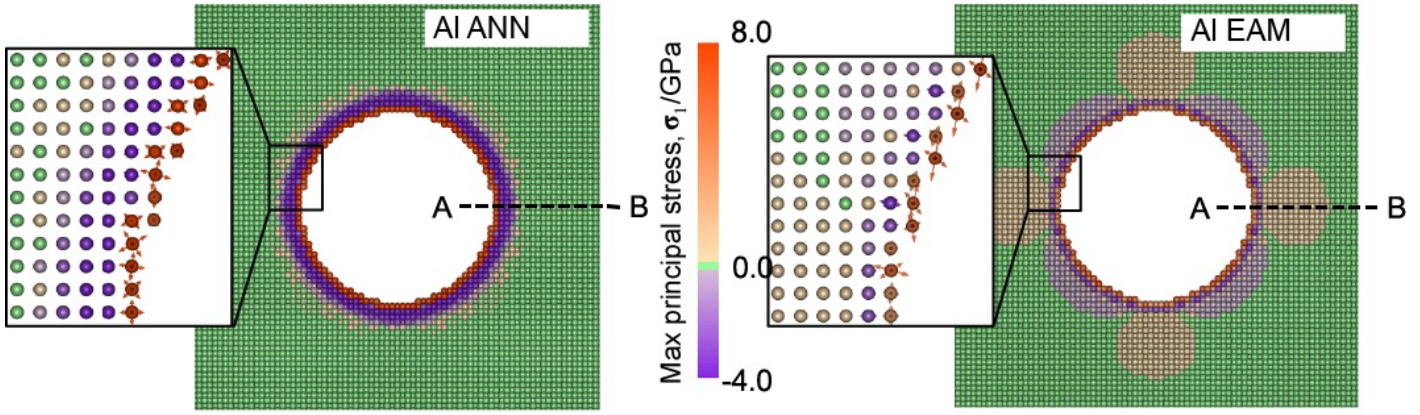
Results: crack propagation on GB

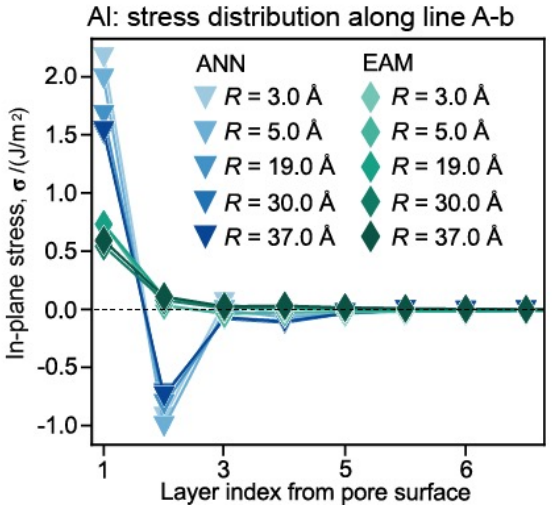


Atomic stress calculation on MLP









Atomic stress fluctuated by quantum effect was firstly unveiled in large systems.

I. Lobzenko, Y. Shiihara, et al., Materials Transactions (accepted)