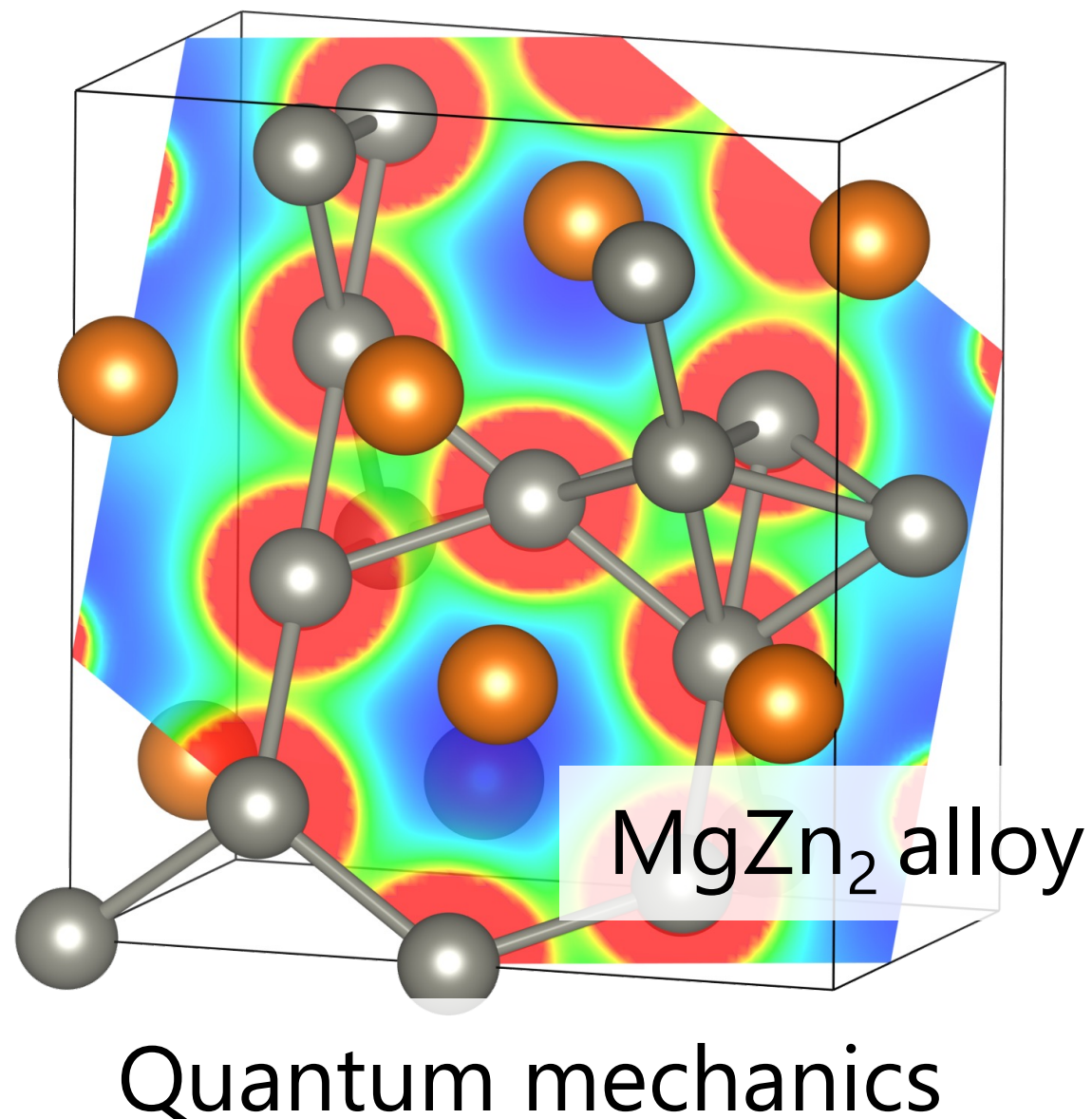
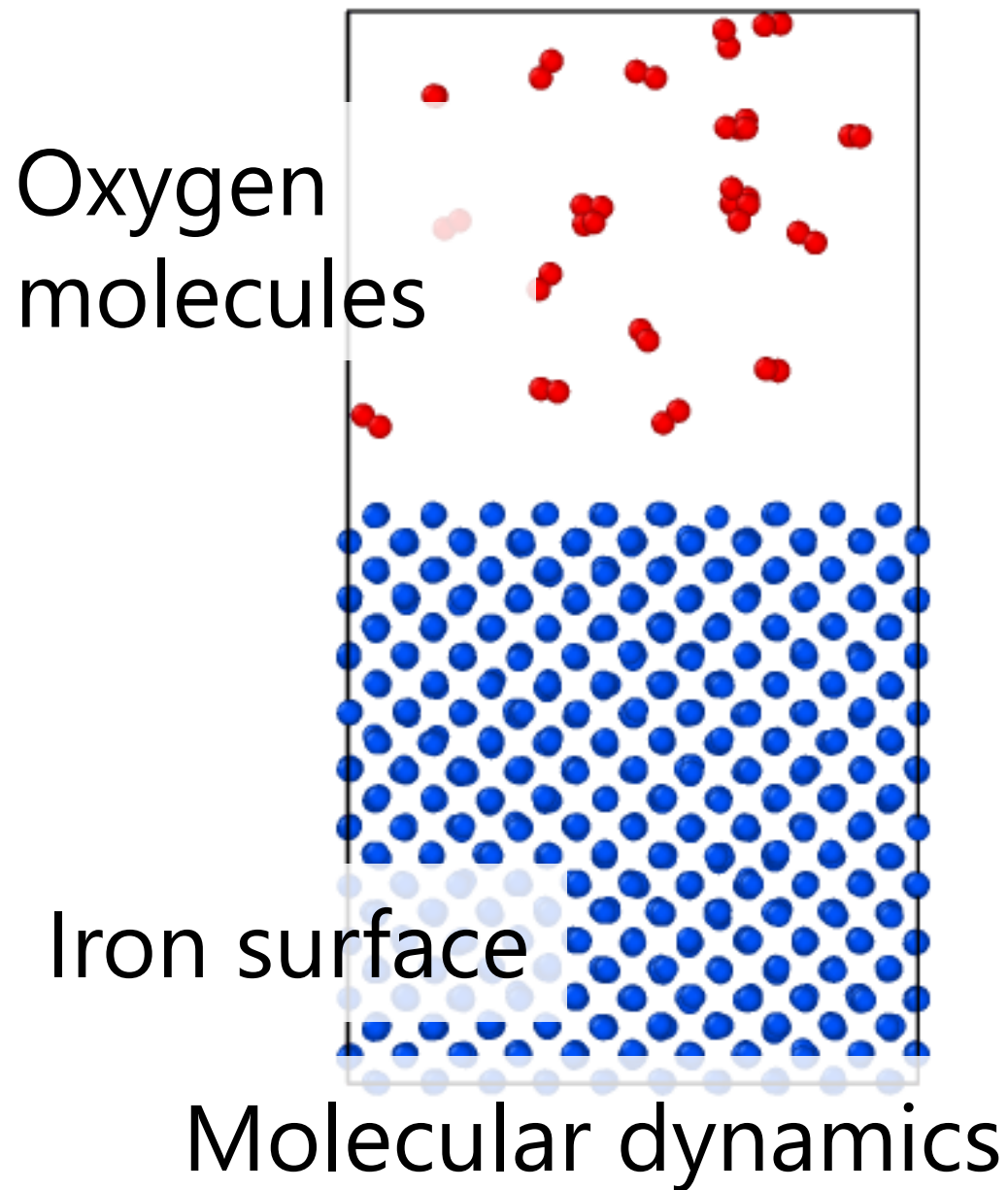


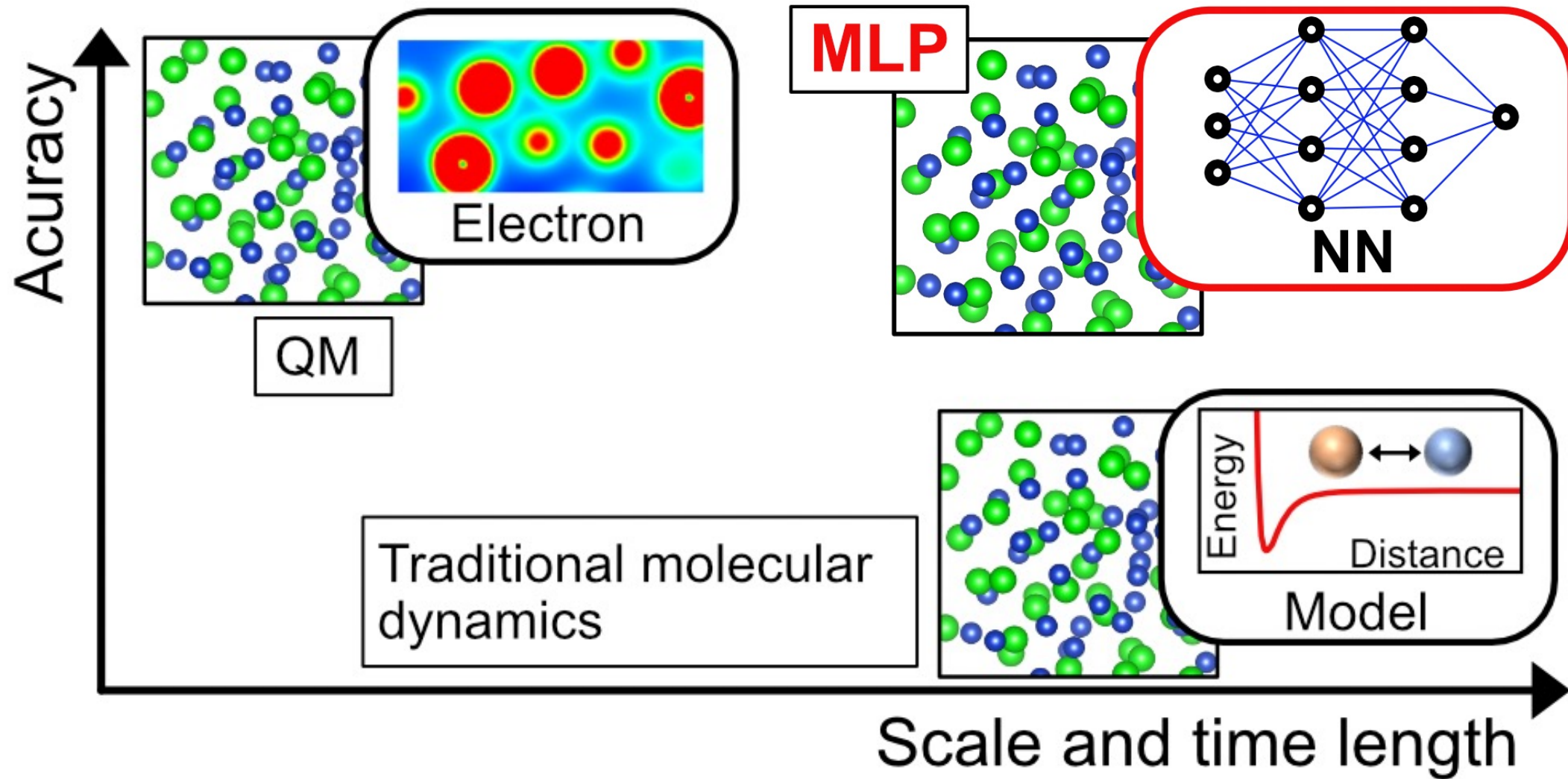
Atomic simulation based on
machine learning techniques:
application to material strength
problems

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Toyota Technological Institute

Simulations of atomic behavior



Problems in atomic simulations

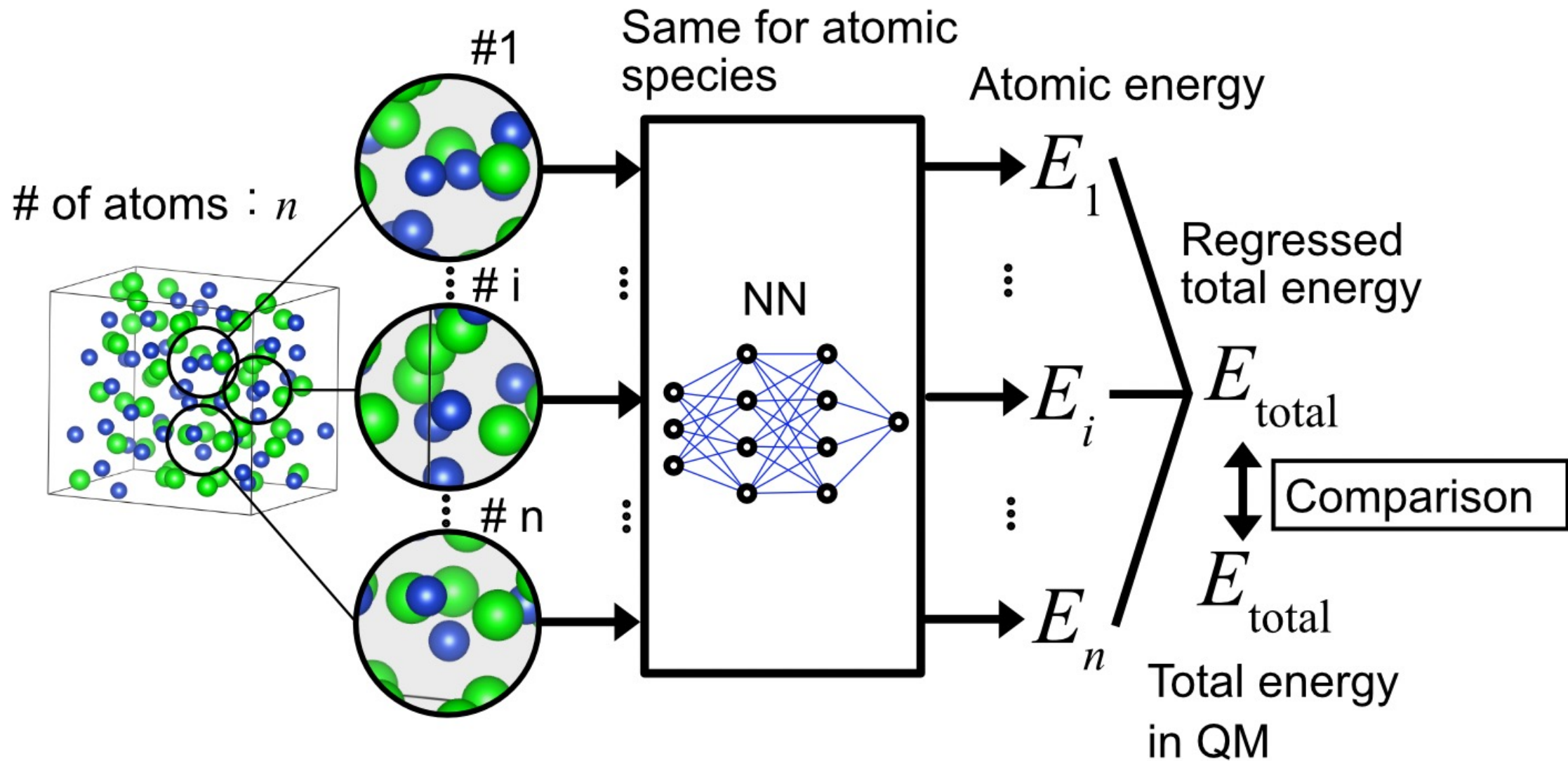


Machine learning is the breakthrough.

A grayscale micrograph showing the grain structure of iron. The grains are irregularly shaped and separated by dark, thick lines representing grain boundaries. The interior of each grain shows a fine, textured pattern, likely due to dislocations or other microstructural features. A white rectangular box is overlaid in the center of the image, containing the text "Application to grain boundary of iron".

Application to grain boundary of iron

Construction of machine learning potential

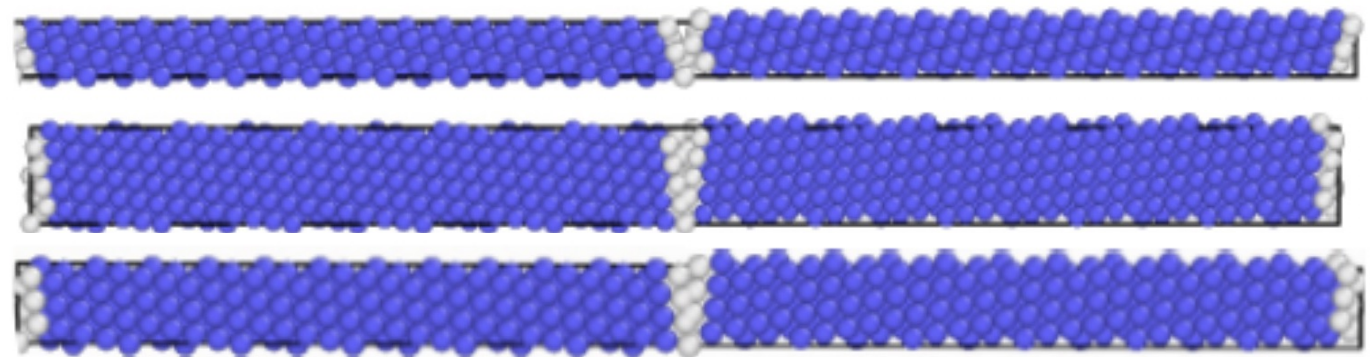
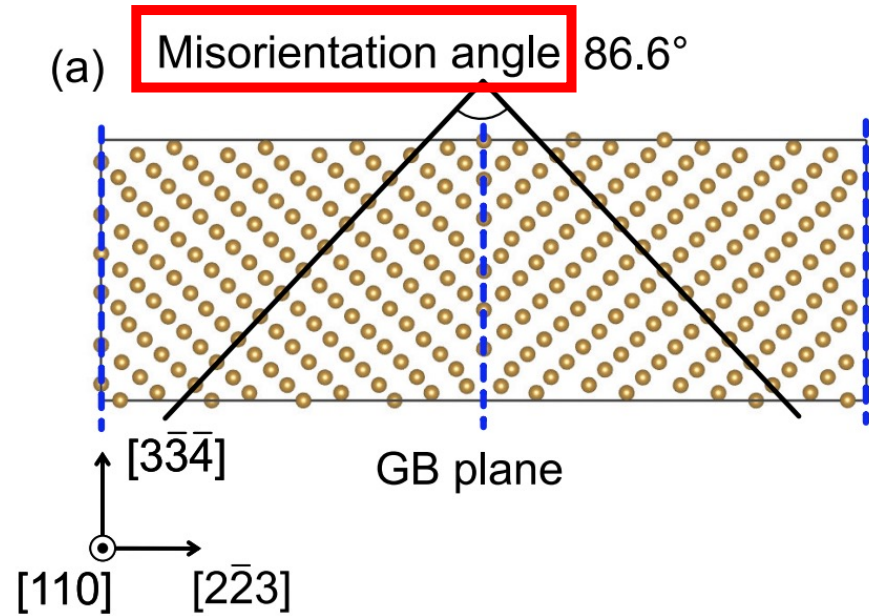
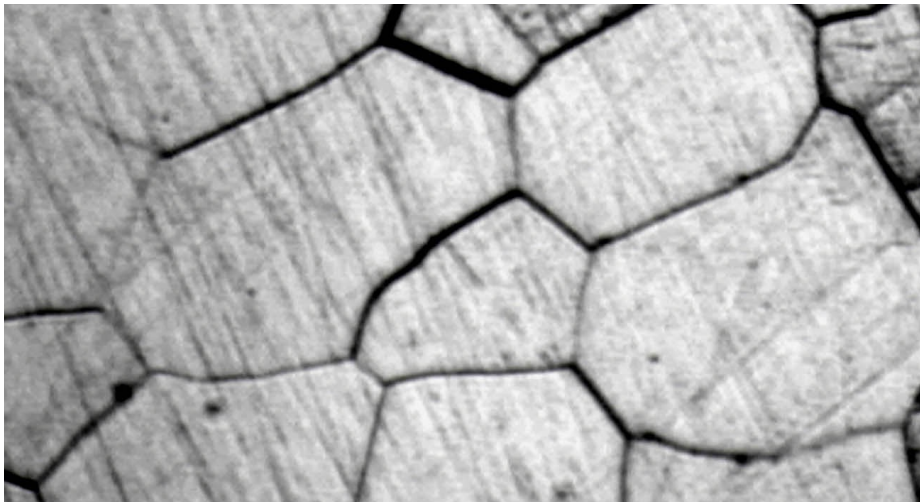


Grain boundary model

Target: calculation of grain boundary energy

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

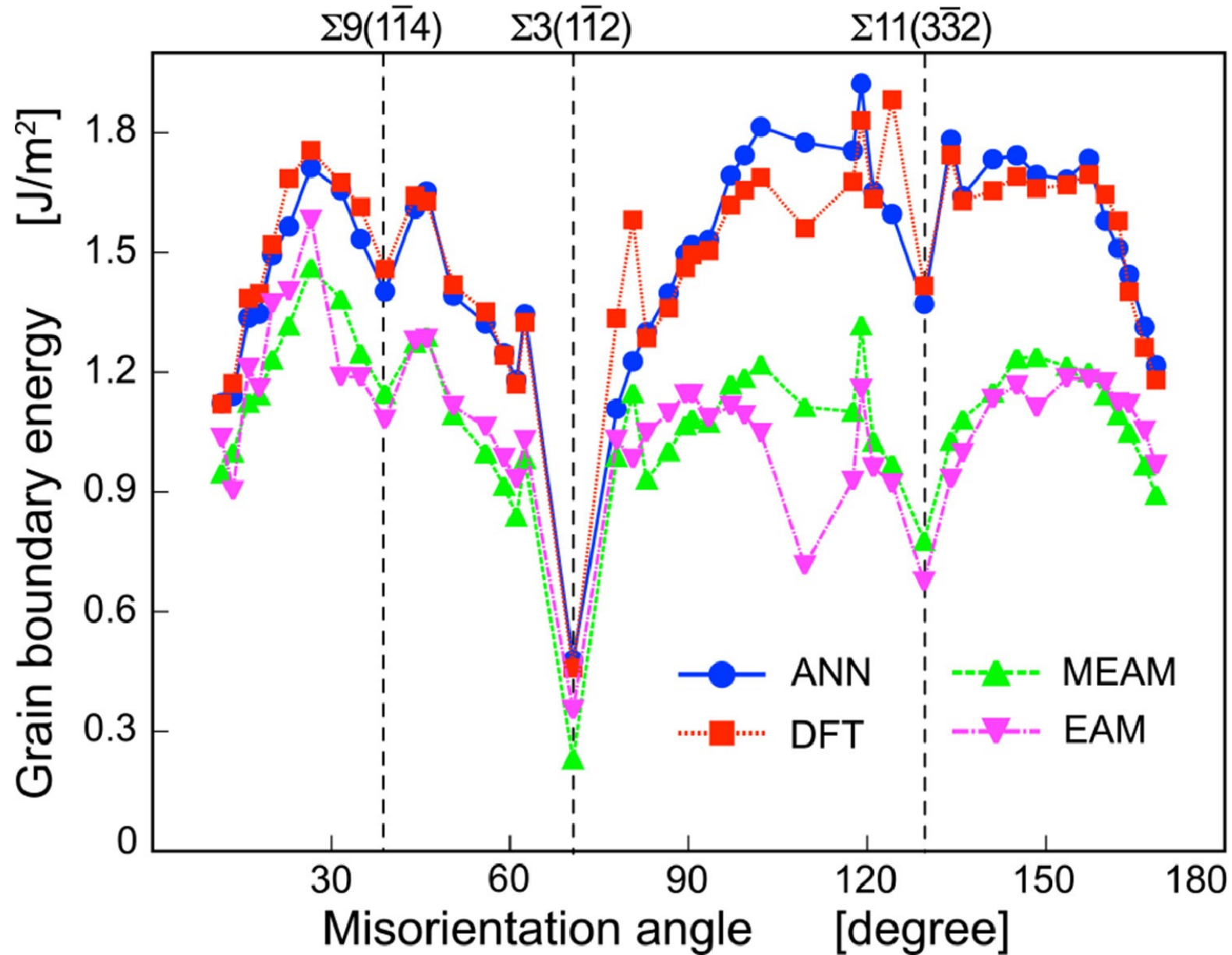
represents stability of GB



...

46 cases with different angles

Results: grain boundary energy



QM and
MLP



Traditional
methods

Results: crack propagation on GB

