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PROCEEDINGS

Effects of Spin Excitation on the Dislocation Dynamics in Body-Centered Cubic Iron

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ABSTRACT

To design the mechanical strength of iron, it is very important to clarify the detail of dislocation dynamics in Body-Centered Cubic (BCC) Iron. The dislocation core structures are typically confined to the nanometer scale.

This implies that the resistance force from discrete atomic columns has a direct bearing on dislocation mobility.

Recently, we've developed a high-fidelity inter-atomic potential leveraging neural networks built upon density functional theory (DFT) data. By conducting dislocation dynamics simulations, we've addressed shortcomings inherent in classical inter-atomic potential approaches. Nonetheless, a significant challenge persists: a three- to four-fold deviation exists between DFT calculations and experimental results regarding screw dislocation mobility.

In this investigation, we're crafting an inter-atomic potential that integrates spin degrees of freedom. With this constructed potential, we aim to explore the impact of Spin Excitation on the dislocation dynamics in BCC iron.

KEYWORDS

Dislocation dynamics; machine learning potential; iron

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