A deep-neural network potential to study transformation-induced plasticity in zirconia

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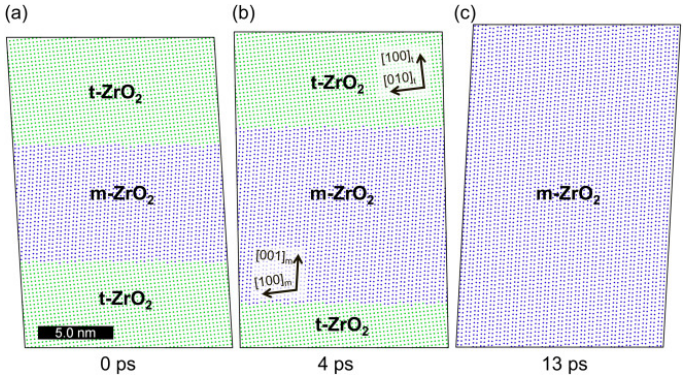
Purpose To develop an efficient interatomic potential accurately representing polymorphism and phase changes of zirconia.

Outline We constructed a novel deep neural network interatomic potential (NNIP) of zirconia using a concurrent-learning approach.

Result The NNIP matches the phase diagrams as well as transformation pathways of zirconia with accuracy comparable to density functional theory.

Computing system:	SQUID GPU nodes
node-hour	500 node-hour
memory used	512 GB
parallelize	1 node



Shear-coupled interface migration of a t-ZrO2/m-ZrO2 interface at 300 K