Energetics of heterogeneous Mg {101-2} deformation twinning migration using an atomistically informed phase-field model

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- An atomistically informed phase-field model for the energetics analysis is constructed.
- A way to introduce the energetics from atomistic simulations to phase-field model is provided.
- General phase transformation with displacive and diffusive modes can be analyzed.
- The energetics of heterogeneous HCP Mg {10-12} twin migration is derived using the model.



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Akio Ishii, "Energetics of heterogeneous Mg f10_12g deformation twinning migration using an atomisticallyinformed phase-field model", Comput. Mater. Sci., 183, 109907, (2020).