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Mesoscale modeling of the martensitic transformations coupled with plasticity in engineering materials

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ABSTRACT

The martensitic transformation (MT) that occurs in several engineering materials, such as steels, Zirconium (Zr) alloys and Titanium (Ti) alloys leads to some interesting material properties. In thisstudy, a physically based 3D elastoplastic phase-field model is developed to study the MT under various thermo-mechanical conditions in single crystals of steel and Zr-alloys. The input data for the model is acquired from different sources, such as CALPHAD, ab initio calculations and experimental measurements. The simulation results clearly show some of the typical characteristics of MT, such as: twinned microstructure formation, autocatalysis, Magee effect (variant selection mechanism under different stress-states), and transformation induced plasticity effect. The study of structure–property relations shows that the stress-states, strain rate as well as the temperature affect the mechanical behavior of steels, giving rise to different yield stresses and hardening behavior. The w phase formation in Zr and the coevolution of mechanical properties are also studied using this model.