Multi-scale modeling of the austenite-martensite transformation in steels

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The austenite-martensite (fcc-bcc) transformation controls the formation of microstructures in a wide range of high strength steels. Recent progress in the physical metallurgy of steels has shown that nanolaminate austenite/martensite microstructures contribute to high material toughness and resistance to hydrogen-embrittlement [1,2]. Despite its relevance for applications, there is no established theory for the transformation capable to predict the contribution of the austenite-martensite phase transformation to ductility.

To clarify the mechanism of transformation, we have performed atomistic simulations of the interface reproducing the major experimental TEM and HRTEM observations in Fe alloys. The atomistic model reveals for the first time the structure and motion of the athermal and glissile fcc austenite/bcc martensite interface in steels [3]. The model shows that fcc to bcc transition is intrinsically athermal, while reverse transformation is not [4]. Furthermore, simulations show that interface motion is activated according to a Schmid-type law, providing an atomic-scale justification of the Patel-Cohen criterion [5].

The atomistic findings have guided the formulation of a new, predictive theory of martensite crystallography. The theory has been incorporated in a continuum, two-scale crystal plasticity model which has been applied to predict the micro- and macro-scale deformation response of lath martensite in FeC steels [4]. The theory has been also validated against High Resolution Digital Image Correlation (HR-DIC) measurements of the transformation in FeNiMn alloys [6], showing quantitative match with experimental measurements of the in-situ transformation strain. Theory predictions show that the fcc/bcc lattice parameter ratio is the key factor controlling the shape deformation (i.e. the in-situ transformation strain), which can achieve more than 90%, namely three times the existing experimental estimates. The theory can thus be used for guiding design of novel and tougher advanced high-strength steels.

References


