In this presentation, we will describe atomistic simulations that predict the kink-pair activation enthalpy as a function of stress in BCC iron that is able to accurately represent the strain rate and temperature dependent plasticity for single crystals. These results are integrated into a crystal plasticity finite element model of BCC iron that captures the deformation of polycrystals and ultimately are used to predict continuum yield surfaces. Our results show that the behavior of polycrystalline BCC iron yield surfaces quickly converges to the standard Von Mises yield surface as temperature increases above 0K. The role of deformation twinning, which is active at low temperature and high rates, is also discussed in context of physically based constitutive models.

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