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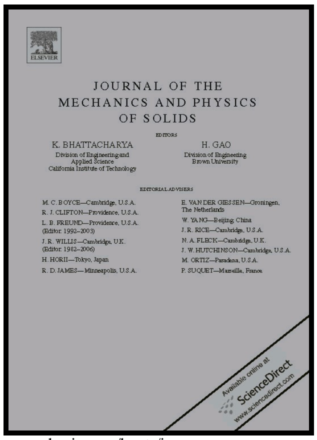

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Abstract

The purpose of the current work is the theoretical and computational comparison of selected models for the energetics of dislocation dissociation resulting in stacking fault and partial dislocation (core) formation in fcc crystals as based on the (generalized) Peierls-Nabarro (GPN: e.g., Xiang et al., 2008; Shen et al., 2014), and phase-field (PF: e.g., Shen and Wang, 2004; Hunter et al., 2011, 2013; Mianroodi and Svendsen, 2015), methodologies (e.g., Wang and Li, 2010). More specifically, in the current work, the GPN-based model of Xiang et al. (2008) is compared theoretically with the PF-based models of Shen and Wang (2004), Hunter et al. (2011, 2013), and Mianroodi and Svendsen (2015). This is carried out here with the help of a unified formulation for these models via a generalization of the approach of Cahn and Hilliard (1958) to mechanics. Differences among these include the model forms for the free energy density ψ_{ela} of the lattice and the free energy density ψ_{sli} associated with dislocation slip. In the PF-based models, for example, ψ_{ela} is formulated with respect to the residual distortion $\boldsymbol{H}_{\mathrm{R}}$ due to dislocation slip (e.g., Khachaturyan, 1983; Mura, 1987), and with respect to the dislocation tensor curl $\boldsymbol{H}_{\mathrm{R}}$ in the GPN model (e.g., Xiang et al., 2008). As shown

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