A comparison of the phase field and Monte Carlo simulations of the interaction between a grain boundary and a coarse particle*

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The paper presents large scale, three-dimensional, Potts model simulations of the interaction between an initially straight grain boundary driven by a bulk stored energy difference across the boundary and a coarse grain boundary particle. The Potts model simulations show that the interaction energy is significantly affected by the choice of the lattice temperature and the driving force. The boundary velocity responds appropriately to changes in the magnitude and direction of the driving force only at high lattice temperatures or high driving forces where the boundary is flexible enough to bend locally near the particle. At lower lattice temperatures or low driving forces, the boundary response is "stiff" and this leads to an increase in the initial energy before it starts to decrease as the boundary approaches the particle. The Potts model simulations are compared with the predictions of the phase field model under identical initial conditions.

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