Simulating the Interaction between a Straight Boundary and a Particle[1]

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Abstract. The paper describes large scale, three-dimensional, Potts model simulations of the interaction between a coarse particle and a straight boundary driven by a bulk stored energy difference across the boundary. It is shown that the variation of the interaction energy as a function of the interface position is significantly affected by the choice of the lattice temperature. The maximum force offered by the particle on the grain boundary decreases with increasing lattice temperature and approaches the theoretical limit at high lattice temperatures. The boundary velocity responds appropriately to changes in the magnitude and direction of the interaction force only at high lattice temperatures.

Introduction

Coarse, incoherent particles offer a drag to the motion of grain boundaries because of the interaction between the boundary and the particle. Since the total boundary energy decreases because of the loss of the boundary area equal to the cross-sectional area of the particle, a boundary that contacts the particle is initially attracted to the particle. As the boundary tries to leave the particle, a pinning force is generated that opposes the driving force. In order to break the boundary away from the particle, a driving force greater than the pinning force is required. The maximum pinning force depends on the particle radius, r, and the interfacial energy per unit area of the boundary, γ, according to [1]

$$F_{\max} = \pi r \gamma . \qquad (1)$$

In the past there have been several attempts to simulate the interaction between a curved boundary and an incoherent particle. Couturier et al [2] used three-dimensional finite element simulations to capture the interaction between a spherical boundary and a particle. The simulations clearly showed the acceleration of the boundary as it contacted the particle, and the deceleration as it attempted to exit the particle. At low driving forces, the boundary velocity approached zero, indicating the complete pinning of the boundary by the particle. Miodownik et al [3] used Potts model simulations and showed that the interaction between the particle and grain boundary is correctly captured only at lattice temperatures high enough to eliminate the faceting of the grain boundary when it interacts with the particle. Carrying a high enough lattice temperature promotes the formation of boundary roughness which results in a transition from a pyramidal to hemispherical morphology of the boundary in the vicinity of the pinning particle.

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The critical lattice temperature above which such a transition occurred was shown to be kT=2.0 for a simple cubic lattice.

In Potts model simulations involving curved boundaries, boundary facets exist inherently on the boundary because of the regular geometry of the lattice. However, the presence of facets on a straight boundary depends on the inclination of the boundary plane. If the boundary is parallel to a symmetry direction, there will be no facets on the boundary. Therefore, the choice of the lattice temperature is far more critical in correctly capturing the interaction between an incoherent particle and a high-angle grain boundary. The current simulations show that lattice temperatures as high as kT=6.0 are required in this case.

Simulations

Monte Carlo simulations were carried out in three dimensional simple cubic lattice using a lattice size of 200 × 200 × 400 sites. The simulation methodology is described elsewhere and will not be repeated here [4]. A coarse particle of radius 40 lattice units was placed at the center of the simulation domain. Periodic boundary conditions were used in all three lattice directions. The straight boundary was driven by a bulk stored energy difference of 0.05 per lattice site. Simulations were carried out at lattice temperatures of kT= 2.5, 3.0 or 6.0. At lower lattice temperatures, the boundary did not move, or moved extremely slowly because of the inability to nucleate a large fraction of steps on the boundary. The position of the boundary and the total boundary energy were tracked as a function of the simulation time. The simulations were repeated with different seed values for the random generator used in the Monte Carlo code, and the results shown represent an average of several runs. The simulations made use of the massively parallel computing facilities at the Oak Ridge National Laboratory.

Results and Discussion

Fig. 1 shows the interaction energy, and force between a flat boundary lying parallel to a lattice symmetry direction driven by a bulk stored energy difference and a particle, and the resulting boundary velocity for a lattice temperature of kT=6.0. As shown in fig. 1a, the boundary energy remains constant prior to interaction with the particle as the boundary remains straight. As it interacts with the particle, boundary energy decreases abruptly as the cross-sectional area that is consumed by the particle increases. In fig. 1 and in subsequent figures, the distance is plotted in units of s/r where s is the average position of the boundary segment that lies within a distance 25 % of the particle radius from the particle surface, and r is the particle radius. The average position is measured relative to the center of the particle.

The normal force on the boundary obtained by taking the derivative of the energy curve with respect to s/r is shown in fig. 1b. The force in fig. 1b and in subsequent figures is shown in terms of $\pi r\gamma$ which is the maximum theoretical drag force exerted by a precipitate of radius r. There is a strong attractive force as the boundary starts to interact with the particle. At this stage of the interaction, there are two competing effects that determine the net boundary energy: (1) the loss in energy due to loss of boundary surface area and (2) the increase in boundary area as it bends towards the particle as shown in fig. 2 which shows the shape of the boundary at various distances from the particle as it moves through the particle. The attractive force increases in magnitude and reaches the maximum very quickly, but the magnitude starts to decrease as the increase in energy due to boundary bending becomes more significant. At a location close to the center of the particle ($s/r \approx 0$) the boundary energy becomes minimum at which point the net force on the boundary is zero. As the boundary starts to come out of the particle, (*s/r* > 0) the energy starts to increase as the negative contribution from loss of surface becomes lower and lower and the positive contribution from bending also increases. Consequently, the force becomes positive, and reaches a maximum value corresponding to *s/r* ≈ 1.0. The contact angle at this point is roughly 45° in accordance with the theoretical value. Beyond this point, the energy increases at a lower rate because the boundary bending close to the particle causes the loss of surface energy by continuing to establish a contact with the boundary even though the undistorted boundary is well beyond the edge of the particle. As the boundary bending becomes more significant and the loss of area becomes insignificant the energy becomes higher than the starting value (s/r ≈ 1.8). As the boundary moves further, it breaks away from the particle, and the energy drops gradually to the original value. During this time the force drops to zero.

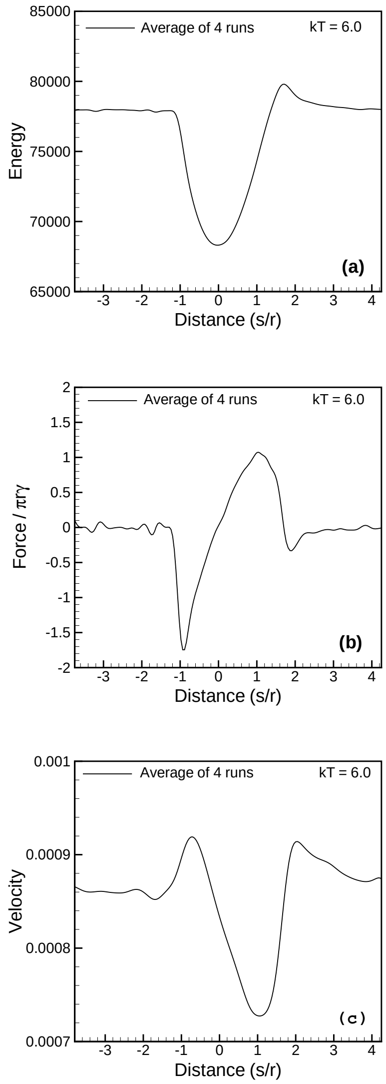

Fig.1. Energy, force and velocity of a flat boundary interacting with a particle at *kT*=6.0.

The above detailed description of the variation of energy and force is in close agreement with theoretical predictions [5]. Fig. 1c shows the velocity of the boundary as a function of *s/r*. The boundary velocity is given by *MF* where *M* is the mobility and *F* is the driving force. Initially, the boundary is moving at a constant velocity as it is driven by a constant force due to the bulk stored energy difference across the boundary. When the boundary experiences an additional force, it responds by increasing or decreasing its velocity proportional to the new driving force. When the boundary approaches the particle, the attractive force due to interaction adds to the driving force and therefore the velocity increases. When the interaction force is repulsive it opposes the original driving force, and therefore the boundary velocity decreases. When interaction force becomes zero as it transitions from attractive to repulsive force, the boundary velocity reaches the original value. Therefore the boundary is quickly able to respond to the changes in driving force due to boundary-particle interaction.

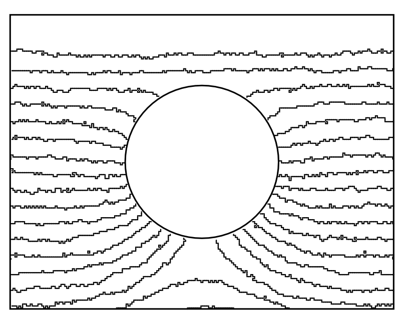

Fig. 2. Boundary shape at various distances from the particle for kT=6.0.

Fig. 3 shows the variation of boundary interaction energy, force and velocity as a function of *s/r* for *kT*=3.0. The energy curve shown in fig. 3a is very similar to the one for *kT*=6.0. However, there is a small hump in the curve just beyond *s/r* ≈ -1, just after the boundary contacts the particle. Fig. 4 shows the shape of the boundary at various distances from the particle for *kT*=3.0. An important difference between fig. 4 and

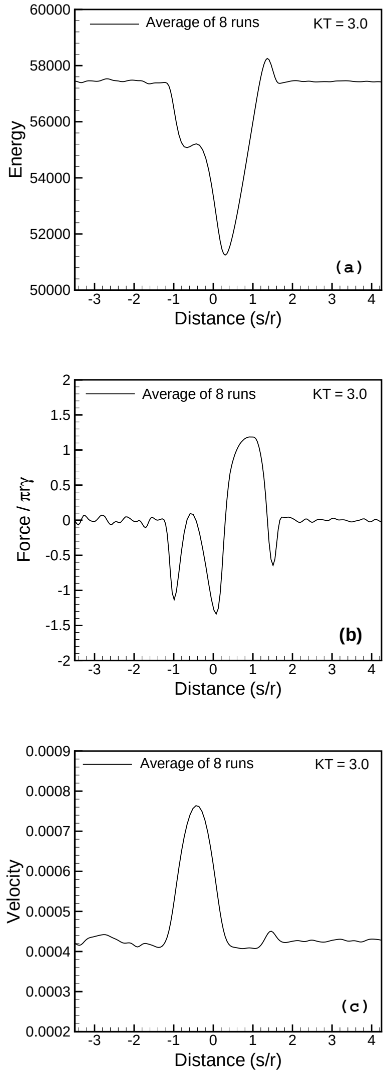

Fig.3. Energy, force and velocity of a flat boundary interacting with a particle at *kT*=3.0.

fig.2 that shows the boundary shapes for *kT*=6.0 is the initial roughness of the boundary. The initial density of steps on the boundary for *kT*=6.0 is significantly higher than for *kT*=3.0. When the boundary interacts with the particle, the roughness increases for *kT*=3.0 because the bending of the boundary towards the particle requires boundary steps to be formed. However, the roughness remains fairly constant for the boundary at *kT*=6.0. The increased roughness of the boundary causes the energy to increase for *kT*=3.0. The increased boundary roughness is particularly significant in the *s/r* range of -1 to 0.5 where the hump in the energy curve in figure 3a is seen. There is also a shift in *s/r* at which the energy is a minimum. While the energy minimum occurs at *s/r* =0 for *kT*=6.0, it occurs at *s/r* =0.4 for *kT*=3.0. This is again due to the differences in the boundary roughness and the differences in the overall bending of the boundary between the two cases.

The variation of interaction force with *s/r* for *kT*=3.0 is shown in fig. 3b. The main difference between fig. 3b and 1b that shows the force versus *s/r* for *kT*=6.0, is that the attractive force decreases in the *s/r* range of -1 to 0.5 where the energy curve shows a positive hump before it starts to increase. The minimum in the force curve at $s/r \approx -1$ is significantly lower for *kT*=6.0 (-1.65) than for *kT*=3.0 (-1.3). The force curve for *kT*=3.0 shows a second minimum at $s/r \approx 0$ (-1.3) which is absent for *kT*=6.0. The second minimum is due to the fact that as the boundary approaches the center of the particle, it becomes smoother once again and the loss of roughness manifests as a fall in energy which results in a negative force. The maximum in the force curve that corresponds to the drag force exerted by the particle on the boundary is very close to the theoretical value for *kT*=6.0 (1.1) while it is somewhat higher for *kT*=3.0 (1.2). The detachment of the boundary from the particle which roughly corresponds to the maximum in the energy curve occurs at *s/r* = 1.8 for *kT*=6.0 and 1.3 for *kT*=3.0.

There is also a significant difference between the velocity versus *s/r* curves for the boundary at *kT*=6.0 and *kT*=3.0 as shown in figs 1c and 3c. Note that there is no good correlation between force and velocity for *kT*=3.0. While the velocity increases as the attractive force increases at $s/r \approx -1$, a decrease in the attractive force does not cause a drop in the boundary velocity in the *s/r* range of -1 to 0.5. In fact, the maximum in the boundary velocity occurs at $s/r \approx -0.5$ when the force on the boundary is zero. After this, the velocity

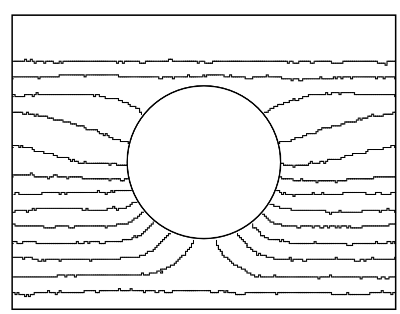

Fig. 4. Boundary shape at various distances from the particle for *kT*=3.0.

drops while the attractive force increases in magnitude. Beyond *s/r* = 0.4, when the positive drag force increases, the velocity does not decrease below the initial value.

These observations clearly indicate that for *kT*=3.0 the relationship between boundary velocity, driving force and boundary mobility are more complicated than for *kT*=6.0. One reason for this behavior is the change in the boundary roughness as the boundary interacts with the particle. During the attractive phase of the interaction, the increase in boundary energy due to increased boundary roughness decreases the overall driving force. However, there is also an increase in the boundary mobility because the mobility is enhanced by the presence of steps. The significant increase in the boundary mobility results in a higher boundary velocity at a lower driving force. Beyond *s/r* = 0.4 when the force becomes positive (drag force) the boundary velocity does not decrease significantly because the boundary becomes relatively smooth and its mobility is extremely low and therefore it does not respond to the decreasing driving force.

The above discrepancies become even more marked at *kT*=2.5 as shown in fig. 5. The boundary shape at various locations of the boundary is shown in fig. 6. The positive hump in the energy curve shown in fig. 5a due to the roughening of the interface is so overwhelming that the energy initially increases and does not begin to drop until *s/r* = -0.5. Between *s/r* ≈ -1 and *s/r* = -0.5, the velocity shown in fig. 5c increases even though there is a positive drag force shown in fig. 5b which is mainly due to the roughening of the boundary. This is similar to the *kT*=3.0 case where the rough boundary, with an increased mobility moves faster although it is now driven by a lower driving force. As in fig 3 for *kT*=3.0, the velocity does not decrease below the initial value when the drag force becomes positive beyond *s/r* =0.2.

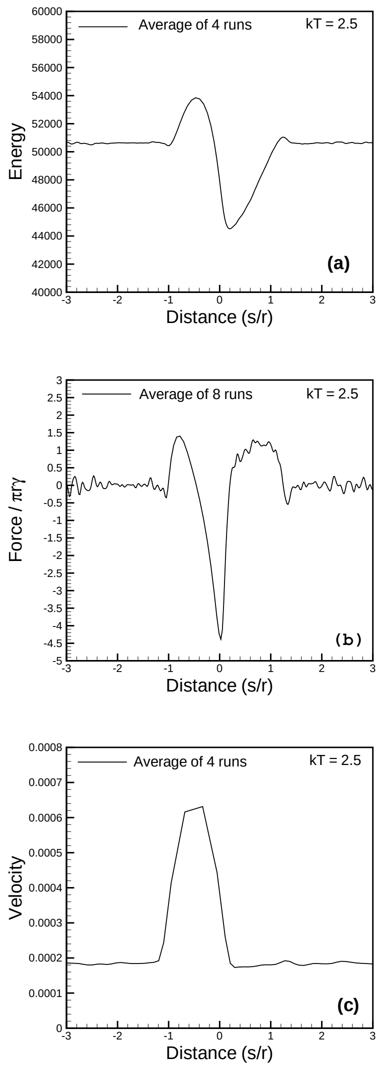

Fig.5. Energy, force and velocity of a flat boundary interacting with a particle at *kT*=2.5.

The importance of choosing the proper lattice temperature in Monte Carlo simulations has been emphasized previously in simulations of stored energy driven interface migration [5], abnormal grain growth [6] and in the interaction between a curved boundary and the particle [3]. In the case of stored energy driven migration, the it is possible to recover the assumed model input values of interfacial energy and

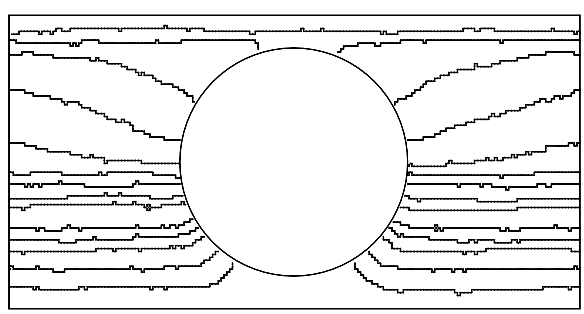

Fig. 6. Boundary shape at various distances from the particle for *kT*=2.5.

mobility from the simulation output only when the lattice temperature used in the model is above a critical value. In the case of abnormal grain growth [6], boundary facets parallel to lattice symmetry directions are formed when sufficient lattice temperature is not used in the model. In the case of the interaction between a curved boundary and a particle, Miodownik et al [3] showed that a minimum lattice temperature of kT=2.0 should be used. In fact, they obtained essentially the same force versus *s/r* curve for kT values of 1.0, 2.0 and 3.0. However, the present simulations show that there are several important differences in the force versus *s/r* curve and velocity versus *s/r* curve up to kT=6.0 in the case of the interaction of a straight boundary with a particle. Interestingly however, the maximum drag force obtained at these various kT values is roughly the same.

Summary and Conclusions

The interaction between a flat boundary and a coarse, incoherent precipitate was simulated using a three-dimensional Potts model. The flat boundary was driven by a bulk stored energy difference across the boundary. The boundary was parallel to a symmetry direction in the simple cubic lattice. The appropriate choice of the lattice temperature for the Potts model simulations was found to be kT=6.0 or higher. At such high lattice temperatures, the boundary roughness remained constant during the interaction of the boundary with the particle, which resulted in the correct estimation of the interaction energy and the drag force. The interface velocity was found to be proportional to the net driving force. At lattice temperatures of kT=3.0 and kT=2.5, the initial boundary was relatively smooth, while the boundary developed steps during the interaction with the precipitate. The increase in boundary roughness resulted in a decrease in the driving force and an increase in the boundary mobility that resulted in an inaccurate estimate of the drag force and the velocity response.

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