A novel Monte Carlo (MC) model of Zener Pinning has been developed. It differs from previous MC models in that it does not simulate polycrystalline grain growth. Instead a single boundary moving through an array of particles is simulated. The boundary curvature defines the driving force acting on the boundary; this is constant throughout the simulation. By incrementally increasing the volume fraction of particles, the pinning force is gradually increased. The boundary is eventually pinned when driving force equals the pinning force. This defines the Zener criterion and enables the volume fraction dependence of the model to be determined. The value of this approach is that there is no limit imposed on either the volume fraction of particles or their size. Simulations have been carried out over a range of volume fractions, from $0 < f < 0.25$ for particles with volumes of 27 sites.

The pinning force exerted by particles on a boundary is related to the characteristic shape during bypass, the so called 'dimple'. When the simulation temperature is $T'=0$, dimples are not formed, the boundaries experience an artificially strong pinning force and the model exhibits an $f^{-1/2}$ dependence. When $T'$ is greater than a critical value dimples are formed and the model shows an $f^{-1}$ volume fraction dependence. The implications of this result for previous MC models of Zener pinning is discussed.
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Introduction

Theoretical analysis [1,2] of Zener pinning gives a relationship between volume fraction of particles, \( f \), their average radius, \( r \), and the final grain size, \( R \). This is expressed as follows:

\[
R = \frac{kr}{\beta f^n}
\]

where \( n \) and \( k \) are constants and \( b \) is function of \( R/r \). The analytical solution gives \( n=1 \), although it is only valid for small values of \( f \) [3,4,5].

Although much experimental work has been carried out, individual experiments rarely provide data over a large range of particle volume fractions. For this reason superposition of data from various sources has been the dominant form of experimental determination of \( n \), and the results are ambiguous [3,6]. Monte-Carlo modeling of the Zener pinning of grain growth in 3D has been carried out by a number of authors [3,7,8]. In all cases \( n = 1/3 \) is found. At small volume fractions, \( f < 0.01 \), the computer results become unreliable with the grain diameters losing an \( f \)-dependence [3]. This is to be expected as the grain size approaches that of the limit of the modeling volume, typically 100x100x100 sites. Thus we have a situation where the analytical models are only valid for small \( f \) which is exactly the regime where the Monte Carlo models become invalid.

To overcome this we need to increase the size of the model, ideally by an order of magnitude to say 1000x1000x1000. The computational time scales with order \((N/P)\) where \( N \) is the number of boundary sites and \( P \) is the number of processors. However there is also a kinetic effect; boundary velocities are inversely proportional to boundary curvature, so as the size of the grains increase we decrease the rate of microstructural evolution. The combination of these two factors means that the only practicable way of running such simulations would be to use a large parallel machine.

There is an alternative approach to increasing the size of the model. This is to increase the scale of the model by modeling a single boundary moving through an array of particles, instead of modeling the whole domain structure. It is this approach we consider in this paper.

The Model

The Monte Carlo Potts model for the simulation of normal grain growth has been described in detail by a number of authors [9,10]. The initial microstructure is mapped onto a 3D simple cubic lattice of variable dimensions \( N_x \times N_y \times N_z \), where each lattice site is allocated a spin number so that all sites within a grain have the same spin. The total system energy is specified by the Potts Hamiltonian:

\[
H = E_0 \sum_{i=1}^{N} \sum_{j=1}^{k} 1 - \delta(s_i, s_j)
\]

where \( E_0 \) is a positive constant defining the energy scale of the simulation, \( s_i \) is the orientation (spin) of site \( i \), \( \delta \) is the Kronecker delta function, and the summation is taken over the \( k \) sites within the neighbour shell of site \( i \) and for all \( N \) lattice sites.
Domain growth kinetics were simulated with Glauber dynamics using first, second and third nearest neighbours on a cubic lattice. The probability \( P(\Delta E) \) that the site will change orientation is calculated from the transition probability function:

\[
P(\Delta E) = \begin{cases} 
1 & (\Delta E \leq 0) \\
\exp[-\Delta E / kT'] & (\Delta E > 0) 
\end{cases}
\]

(3)

where \( T' \) is the simulation temperature and \( k \) is a constant. A spin change is always accepted if it decreases the local energy of the site. If it increases the local energy it is accepted according to an Arrenhius probability. \( T' \) is not a real temperature. It simply alters the transition probability function, equation 3. Using \( T' = 0 \) ensures that only events that lower the local interfacial energy of the system are allowed.

The model used in this study is not strictly a Potts model since it only selects boundary sites for spin flips. Thus it does not allow nucleation of new sub-grains even when \( T' > 0 \).

Hexag Boundaries

A novel geometry was used to simulate the kinetics of a boundary moving under a constant driving force. This geometry consists of a planar grain on top of an hexagonal boundary network shown in figure 1. The hexagonal boundary network is static throughout the simulation since all the boundaries intersect at 120°. Only the boundary between the planar grain and the hexagonal grains is in a non-equilibrium state which causes the planar grain to migrate in the negative z direction. The driving force is provided by the consumption of the hexagonal grains by the planar grain. Since the geometry of the hexagonal grains is static, this driving force is constant. The magnitude of the driving force is determined by the size of the hexagonal grains, characterised by the grain size \( D \), see Figure 1.

The kinetics of hexag boundaries is discussed in detail by Miodownik, Martin and Cerezo [11]. They report that the boundaries migrate via a ledge mechanism. Crucially they find that ledge repulsion exists if \( kT' < 2 \) and so the boundaries only exhibit a constant mobility independent of curvature when \( kT' \geq 2 \). They also carried out simulations of boundaries interacting with single particles of various sizes. They report that the Monte Carlo model does not simulate equilibrium boundary tension when \( kT' < 1 \), as a result facets, and not dimples, are formed during particle bypass, see figure 2(a), and so the effective pinning forces are very

![Figure 1. The hexag. A vertical network of hexagonal grain boundaries. A grain inserted on top of the hexag experiences a constant driving force.](image)

![Figure 2. Boundary geometry during particle bypass: (a) facets are formed when \( kT' = 0 \) (b) dimples are formed when \( kT' = 1 \)](image)
high. When $kT'>1$, dimples are formed during particle bypass, see figure 2(b) and
the measured pinning force shows good agreement with that calculated
theoretically.

In the current work the simulations were carried out using $kT'>=2$. For each value
of $D$ the $N_x$ and $N_y$ dimensions of the simulation box were varied to preserve
hexagonal geometry. The values of $D$ and their corresponding lattice volumes
were respectively; 10 (20x22x50), 17 (39x34x50), 25 (58x50x50), 50 (116x100x50).
Boundary conditions were periodic in the $x$ and $y$ directions.

For each simulation a volume fraction of particles (3x3x3 cubes) was randomly
inserted into the simulation volume. If the boundary was able to migrate between
$z=10$ and $z=35$, the volume fraction was incremented and the boundary returned to
its initial position. The process was repeated until a volume fraction of particles
was inserted into the lattice which pinned the boundary. The process is illustrated
in Figure 3. Each simulation was repeated ten times for each driving force and
volume fraction.

**Results and Discussion**

The probability $p(f)$ of the boundary being pinned by a particular volume fraction
was defined as the fraction of unsuccessful attempts to migrate through the particle
array. The minimum volume fraction that produced $p(f)=1$ was defined as $f_c$. The
probability functions, $p(f/f_c)$, for each driving force are plotted in figure 4. The plot
can be divided up into three regions. Region I, $f/f_c<0.5$, where the probability that
the boundary will be pinned is zero. Region II, $0.5< f/f_c<1$, where there is a finite
probability that the boundary will be pinned. Region III where the boundary will
certainly be pinned. Despite some scatter, all the data lies on the same curve.

The plot may be explained in the following way: the boundary will experience a
force depending on the number of particles in contact with it. The pinning force
will be dependent on the situation of the particles in contact with the boundary ie.
where they are on the boundary and their distance from the boundary. If a particle
is in front of the boundary it will pull the boundary forward, if it is behind, it will
pull it back. The net pinning force will be the sum of these forces. It is clear that
although the average pinning force will be constant, the actual pinning force at any
point in time will depend on the position of the boundary with respect to the

![Figure 3. Hexag boundary moving through an array of particles.](image)

![Figure 4. Probability of a boundary being pinned as a function of $f/f_c$.](image)
particle topology. Only by using a regular array of particles could we avoid this effect and this would yield a $p(f/f_z)$ which was a step function. By using a random particle array we allow the boundary to experience a range of pinning forces. If the pinning force ever exceeds the driving force the boundary becomes pinned. Hence the existence of Region II, which shows that the probability of this happening is a function of $f/f_z$.

Alternatively we can use a mean field approach to analyse the data. The driving force acting on the simulated boundary is $2\gamma D$ [9]. Assuming a pinning force given by the Zener stress [10]:

$$\sigma_p = \frac{3\beta f\gamma}{4r}$$  \hspace{1cm} (4)

Then the boundary will be pinned when:

$$D_z = \frac{8r}{3\beta f_z}$$  \hspace{1cm} (5)

As expected this equation is identical in form to the expression for the Zener pinned grain size. A plot of $\log(D_z/r)$ against $\log(f)$ is shown in Figure 5. The data cover the range volume fractions, $0.0032 < f_z < 0.24$, and lie on a straight line with a gradient of $n=1.06$. This is close to the value of $n=1$ expected from analytical considerations (equation 1). The discrepancy may be due to the longer particle detachment distances observed in the model by Miodownik, Martin and Cerezo [11]. There may also be additional lattice effects due to the geometry of the hexagonal boundary.

Figure 5 shows data from simulations carried out by Miodownik [12] at $kT'=0$ which give $n=0.59$. Note that in addition to a difference in $n$, the boundaries have much lower values of $f_z$. The data show that at $kT'=0$ the model exhibits strong pinning even when $f<0.01$. This is not surprising in light of the ledge pinning mechanism mentioned previously. Lastly, we would not expect nor do we see any $f$-dependence transition in the model. This is because the arguments for the existence of a transition are based on topological considerations of a domain system [5]. These are clearly not present in the current system.

Conclusions

Zener pinning has been modeled using a single boundary migrating through an array of particles.

The particle pinning force in Monte Carlo simulations is a function of temperature. To model pinning correctly it is important to make sure that simulations of Zener pinning are carried out with the value of $kT'$.
greater than a threshold value. In the present simulation this was $kT' = 2$.

The simulation is in agreement with analytical models that the volume fraction dependence of Zener Pinning is $n = 1$. Previous Monte Carlo simulations carried out at $kT' = 0$ and are believed to exhibit strong pinning due to lattice anisotropy in the simulation.

References

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