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COMPUTER MODELLING OF PARTICLE LIMITED GRAIN GROWTH AND ITS EXPERIMENTAL VERIFICATION.

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ABSTRACT

Data from two simulations on particle limited grain growth are reported. For 3D simulations the same type of strong correlation between particles and grain boundaries previously found in 2D simulations was found with the limiting grain size scaling in 3D with $(1/f)^{0.31}$. Very much higher particle correlation with grain boundaries and particularly with grain corners was obtained than expected for the random microstructure. The size distribution of the pinned grain structures showed considerable differences from that of dynamically evolving single phase structures - notably an absence of small grains with radii less than 0.3 <R> and the presence of a few large grains in the pinned samples. In 2D simulations from a finite starting grain size it was shown that the limiting grain size is strongly modified by the starting grain size which may explain at least part of the wide scatter in pinned grain sizes reported from experimental studies. It is suggested that normal grain growth ceases when the smallest grains in the size distribution can no longer shrink. Finally limited new experimental data on grain growth with a stable dispersion in an Al-Fe alloy is reported. This data is, at least partially, in agreement with the simulation results but most strikingly shows a ready transition to abnormal grain growth at low volume fraction of second phase particles. A simple model for this effect is proposed - based on the Zener analysis but applied only to abnormal grain growth into a fine grain structure pinned to a small grain size in the maner suggested by the simulations.

1. INTRODUCTION

In the 7th Riso Conference, Anderson(1986) described the Monte Carlo simulation technique used to study grain growth. In the early studies, Anderson et al.(1984), Srolovitz et al.(1984a) established how, by use of a 2 dimensional hexagonal lattice, 2D grain growth could be effectively simulated both with respect to kinetics and to the microstructure including the steady state grain size distribution. Subsequent studies by Grest et al.(1988), using a larger lattice and in consequence a longer periods of grain growth, established the expected kinetics, eq.1b with $n = 0.49 \pm 0.02$. The fundamental equation is:

$$\langle R \rangle^m (t) = \langle R \rangle^m (o) + B\,t \qquad (1)$$

Which at long times, $\langle R \rangle^m (t) >> \langle R \rangle^m (o)$, reduces to the usually quoted form:

$$\langle R \rangle (t) = B'\,t^n \qquad (1a)$$

<R> (t) is the mean grain radius at time t. As has been repeatedly shown (Atkinson 1988, Mullins and Vinals1989) in interface controlled reactions involving growth of a "self similar" structure, such as 2 or 3D grain growth, n should be 0.5. In an important recent extension the computer simulation technique was extended to 3D simulation, Anderson et al. (1985, 1989a). They showed in 3D simulations very similar results, initially n = 0.48±0.04 but with a larger lattice and longer times n = 0.47± 0.02 was obtained. As discussed by Anderson et al. (1986 and1989a) the simulations appear to match not only the analytical kinetic behavior but also to match experimental observations of the grain size distributions and the grain topology.

The same type of method has been used to study recrystallization in 2D simulations for both homogeneous nucleation (Srolovitz et al. 1986) and heterogeneous nucleation (Srolovitz et al. 1988). The simulation of homogeneously nucleated recrystallization showed the correct form of the Johnson-Mehl-Avrami-Kolmogorov(JMAK) kinetics. Doherty et al.(1986) in the 7th Riso Symposium used the same type of simulation to explore the problem of of the usual failure to observe the expected JMAK kinetics for recrystallization. It was found that if the stored energy was varied from grain to grain then reduced JMAK exponents were found - very similar to those seen in experimental studies of plastically deformed metals. Further studies by Rollett et al.(1989a) confirmed these results and directly demonstrated that the crucial assumption of the JMAK analysis of nucleation and growth reactions, eq.2, while valid for uniform stored energies was seriously in error for non-uniform stored energy.

$$dF = (1 - F)\, dFe \qquad (2)$$

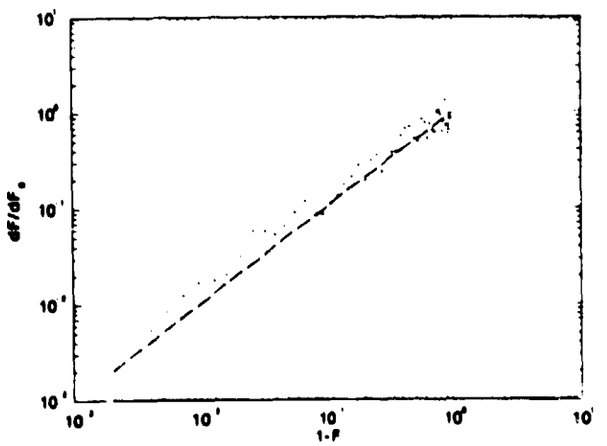


Fig.1. Double log plot of the rate of increase of actual fraction recrystallized, dF, to the extended fraction, dFe, versus 1 - F for uniform stored energy.
From Rollett et al. (1989a).

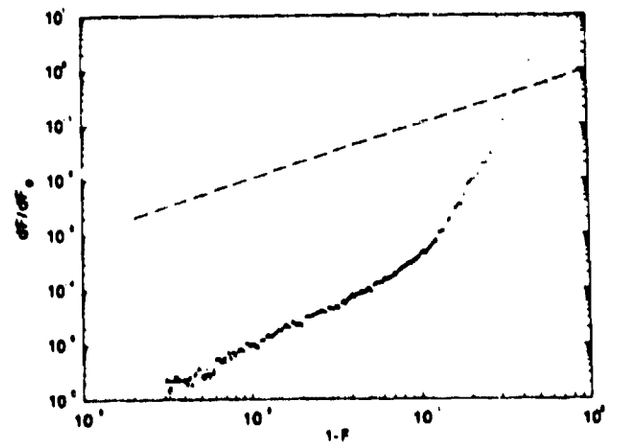


Fig.2. Double log plot of the rate of increase of actual fraction recrystallized, dF, to the extended fraction, dFe, versus 1 - F for non - uniform stored energy.
From Rollett et al. (1989a).

F is the true volume fraction of transformed material and Fe is the extended volume fraction - the volume occupied by the new structure if no correction is made for impingement of the growing

new grains. Fig.1 shows the close agreement to eq. 2 for uniform stored energy where the assumptions leading to eq.2, random nucleation and spatially constant growth, are found. Fig.2 however shows that the with non uniform stored energy the impingement correction is grossly underestimated by eq.2. The physical meaning of this is that in regions of higher stored energy more grains are nucleated and they grow faster into the more deformed grains than elsewhere. As a consequence there is much more impingement occuring amongst these clustered grains than is predicted for a more random structure at the same fraction recrystallized. Such clustering of nuclei in selected grains in moderately deformed pure metals is commonly observed as discussed by Doherty et al.(1986) and Rollett et al.(1989a). Very recently Hutchinson et al.(1989) demonstrated the validity of this concept by elegant residual stored energy measurements during recrystallization. In heavily rolled coarse and fine grain sized copper over 50% of the stored energy was released while the first 20% of the deformed material recrystallized.

In both studies of normal grain growth in single phase materials and of recrystallization the computer simulations seem to match the current analytical models very closely provided that the assumptions of the simulations and the analysis were the same. The recrystallization studies also showed that the simulations could match experimental conditions rather well, at least qualitatively, in much more complex situations. These close matches lend some confidence to the validity of the simulations even though there may remain possible doubts about the validity of the simulation in different circumstances - in all cases simulation like analysis only provides a basis for suggesting and analysing actual experiments.

In the situation of grain growth in particle containing materials the simulation results have been found to give significantly different result from the standard analytical theory and these results including recent new results will be described here and compared with previous experiments and with some preliminary new experimental studies suggested by the simulations.

2. CLASSICAL PARTICLE LIMITED GRAIN GROWTH

The classical analysis was provided by Zener though published by Smith(1948). The subject has been reviewed many times, see Ashby(1980) Nes et al.(1985) Hillert(1988) and only the major assumptions and results need be given here. When a grain boundary migrates onto an spherical incoherent particle of radius r (that is one whose interfacial energy is unchanged by passage of a high angle grain boundary) the system reduces its energy by ΔE:

$$\Delta E = \pi r^2 \gamma \qquad (3)$$

γ is the grain boundary energy. To move the boundary off the particle a force F must be applied and this force achieves a maximum value given by:

$$F = \pi r \gamma \qquad (4)$$

If it is assumed that the boundary and the particles are uncorrelated in position, then the number of particles on unit area of the boundary N is:

$$N = 3f / 2\pi r^2 \qquad (5)$$

Where f is the volume fraction of particles. The product of N and F gives the Zener drag, Z, provided by the particles against the migration of a grain boundary moving under a driving pressure P.

$$Z = NF = 3f\gamma / 2r \qquad (6)$$

By soap film simulations and by studies of recrystallization in particle containing alloys with a stored energy P that fell with distance(from a hardness indent) Ashby et al. (1969) were able to confirm to a surprising accuracy the validity of this simple model. The recrystallized grain boundaries and the pressurised soap films were halted when P = Z. More detailed analyses, see

Gladman (1966), Louat (1982), Nes et al.(1985), Hillert(1988), only changed slightly the results of the simple Zener analysis. There seems at present no reason to doubt the validity of the analysis for migration of a high angle grain boundary between two grains when driven by a pressure P that arises from energy differences between the grains. Current Monte Carlo simulations of recrystallization in 2 dimensional (2D) particle containing structures by Rollett et al. (1989b) seems to support the conclusion that when $Z < P$ in recrystallization the boundaries can migrate past the particles with little difficulty and that there is a random correlation of particles with boundaries so that, the 2D equivalent of, eq. 5 is valid for recrystallization.

A very different result appears however when boundary migration is occuring during grain growth - that is when boundaries experience a pressure P determined by their own radius of curvature, R_c.

$$P = 2\gamma / R_c \qquad (7)$$

Assuming as in the Zener analysis that grain growth will cease when the mean radius of curvature (taken in the simple model to be equal to the mean grain size <D>) increases until $Z = P$ - this gives the much quoted Zener result:

$$\langle D \rangle = 4r / 3f \qquad (8)$$

Again more detailed analysis using the same assumptions only effects this result in a rather marginal way, see Gladman(1966), Louat(1982), Nes et al.(1985), Hillert(1988). An alternative point of view has been expressed, apparently independently, by various investigators: Haroun and Budworth(1968), Anand and Gurland(1975), Hellman and Hillert(1975), Hutchinson and Duggan(1978) and Doherty et al.(1987). In this approach it was either observed directly or predicted that the majority of particles will lie on boundaries between 2 grains or at edges between 3 grains or at corners between 4 grains. Under these circumstances the number density of particles on unit area of grain boundary is much larger than predicted by eq.5 and the limiting grain size is then found to vary with the volume fraction of particles as:

Particles at boundaries: $$\langle D \rangle = k r / (f)^{0.5} \qquad (9)$$

or at corners: $$\langle D \rangle = k' r / (f)^{0.33} \qquad (10)$$

Experimental data supporting eq. 9 has been provided by Anand and Gurland(1975) and Hellman and Hillert(1975) in quench and tempered steels and to a more sophisticated version of eq. 9 taking into account the dispersion of particle radii for grain sizes in sintered calcium flouride by Haroun(1980). Data that gave plausible fit to eq. 10 has been provided by Olgaard and Evans (1986) using their own data for hot pressed calcite and from a reanalysis of a large range of data from both metallic and ceramic materials. The summarized data from the Olgaard and Evans review is shown as fig.3, in which log (D/d) is plotted against log f and trend lines of slopes 1:1 (eq.8), 1:2 (eq.9) and 1:3 (eq.10) are given. Fig.3 indicates several striking features which include:

i) The very large scatter, especially in the ceramic data
Note that "cal" is calcite, Lange and Hirlinger(1984) and Green(1982) are for alumina, in these cases the mixed ceramic powders are blended and hot pressed. The metal data covers recrystallized Al containing fine alumina, Tweed et al. (1983) and the examples of quench and tempered steel, Anand and Gurland (1975) and Hellman and Hillert (1975).

ii) The tendency for almost all individual pieces of data (except that of Hsu) to show a slope closer to eqs 9 and 10 than the 1:1 slope of eq.8. In the table of data published by Olgaard and Evans(1986) this is shown more clearly. However it should be noted that additional data by Koul and Pickering(1982) on grain growth in recrystallized austenitic steels also fits quite closely the results of Hsu (1984).

iii) The simple Zener result clearly fails at very low values of f - the lowest D/d value in Al-Al_2O_3 (Tweed et al.1983) falls nearly two orders of magnitude below the prediction of eq.8.

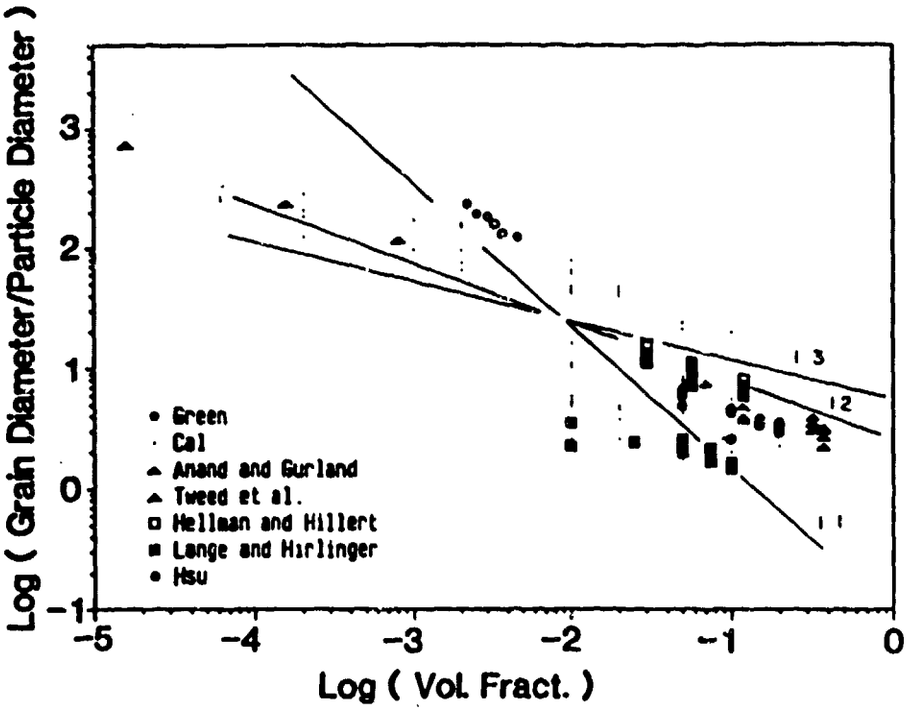


Fig. 3. Log of the ratio of the pinned grain size to the particle diameter versus log of the volume fraction of second phase particles. Lines of slopes 1:1, 1:2 and 1:3 are plotted. From Olgaard and Evans (1986).

It is for this problem that the Monte Carlo simulations are of great value. In a crucial paper Srolovitz et al. (1984b) studied grain growth in 2D with a range of volume fractions between 0.05 and 0.005. The initial "grain size" was a lattice point, the same size as the inert particle, and for much of the growth time the mean growth rate showed no effect of the particles - not surprisingly since most grains were not in contact with any particles. As the grain size reached the approximate interparticle spacing, $S = (1/f)^{0.5}$, the growth rate slowed down and finally halted at a mean grain radius $\langle R \rangle$ given by:

$$\langle R \rangle = (1.70 \pm 0.06)\, r / (f)^{0.5} \qquad (11)$$

The fraction of particles on grain boundaries, ϕ, was found to be close to 1 so that, as discussed by Doherty et al.(1987), under these circumstances eq.9 should be the expected result using the Zener analysis for 2D grain growth. Srolovitz et al. (1984b) had themselves derived eq. 11 on the simple basis that in 2D particles are extremely effective in removing the curvature required for grain growth, so that when each grain is in contact with 3 particles, all grain growth ceases. This immediately gives eq.11 as $\langle R \rangle = (3)^{0.5}\, r / (f)^{0.5}$. Hillert(1988) obtained the identical result - even an isolated triangular grain with 3 particles at its corners will not vanish, fig. 4. However in the same paper the problem of 3D grain growth in the presence of particles was still discussed in the original Zener manner - as a drag on a migrating boundary surface between two grains and not in terms the influence of particles in removing curvature - the analysis which has proved to be so useful in the 2D case.

To gain further insight into this problems two further types of simulation have been run and will be briefly described here: A 3D simulation run from an initial grain size of one lattice point - that is with the initial grain size very much smaller than the interparticle spacing, initial results from that study have been already published in outline, Anderson et al (1989b). In the second type of simulation, run so far only in 2D, grains were initially grown without particles to a mean area $\langle A \rangle_0 >> a$, the particle and lattice site area. At this point different volume fractions of particles were randomly introduced into the microstructure and grain growth allowed to continue until a limiting size was achieved. The point of this simulation was to model the usual case in a metallurgical structure of a grain structure achieved, for example by recrystallization

when the boundaries will rapidly pass particles, so giving a near Zener-like situation of random boundary particle boundary correlation. Grain growth from this type of situation is that commonly seen in metallurgical processing. The development of "ceramic-like" microstructures with two immiscible phases mixed at a grain level with both phases allowed to coarsen has not yet been simulated. In both the current simulations the total fraction of the particles found on all grain boundaries, the separate fractions of particles at boundaries between 2 grains, at 3 grain edges, and in the 3D simulation, the fraction at 4 grain corners, ϕ, ϕ_2, ϕ_3, ϕ_4, were continuously monitored.

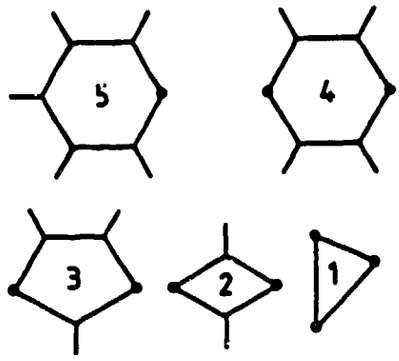


Fig.4. Removal of curvature in 2D grains with less than six neighbours by the presence of particles.
From Hillert (1988).

3. 3D SIMULATION - SMALL INITIAL GRAIN SIZE

The technique has been previously described (see Anderson 1986 and Anderson et al. (1989a and b)) so only a very brief outline need be given. At the start of the simulation each lattice point is given a random number Q, between 1 and 48, and then randomly selected sites have their Q value randomly switched to a different value. The total energy of the system is determined by assigning an energy J between any two lattice points with different Q values. Any switch in Q that lowers the energy, or does not increase it, is accepted. The unit of time is the Monte Carlo Step (MCS) - where 1 MCS is determined by a number of attempted switches equal to the number of switchable lattice points. In the 3D simulation a simple cubic lattice was used with 100x100x100 lattice points and with the first, second and third nearest site neighbours counted as contributing an equal amount, J, to the energy of unlike neighbours. Anderson et al. (1989a) have described the detailed studies of 3D single phase grain growth simulation. In order to simulate the effect of second phase particles at the start of the simulation, when the number of grains is comparable to the number of lattice points, a fraction, f, of points were selected at random and each given a new number, Q + 1. These sites were not allowed to switch. These sites therefor represent second phase particles particles and they were assigned the same energy penalty, J per neighbour, as determined the grain boundary energy. That is the simulated particle / matrix interface has the same interfacial energy as the matrix grain boundaries. The particles were not allowed to move or to coarsen. As in a real structure, when a grain boundary moves onto a particle there is a reduction in energy of the system, eq.3. Different volume fractions of particles were used, from f = 0.005 to f = 0.16, and for each value of f, two runs were performed to improve the statistical averaging. At early times the mean grain volume grew rapidly at the same rate as a particle free microstructure, but as the grains grew to a size comparable to the interparticle spacing, $(1/f)^{1/3}$, the grain growth halted at a limiting grain size, fig.5. Fig. 6 shows sections through the 3D microstructures in the pinned state at two of the volume fractions and fig.7 shows the crucial result of how the mean limiting grain volume V_L, varies with the volume fraction, f, of particles on a log/log plot. The dashed line in fig 7 is the empirical eq.12.

$$V_L / v = k / f^b \qquad (12)$$

v is the volume of one lattice site, $k = 91.0 \pm 16.9$ and $b = 0.922 \pm 0.045$. On reducing eq. 12 to give the limiting grain radii we obtain eq.13.

$$R_L/r = k'/f^c \qquad (13)$$

Here k' is found to be 4.5 ± 0.8 and the crucial exponent, c. is 0.31 ± 0.02. v is the volume and r the radius of one lattice point - that is the pinning particle. This result is the expected form of eq.10, when the grains have grown to a size equivalent to the mean particle spacing, $(1/f)^{1/3}$, that is with most of the particles at grain corners, Hellman and Hillert (1975).

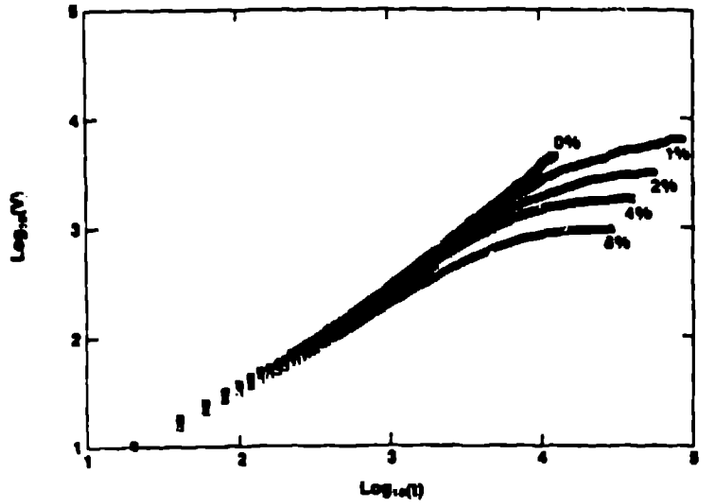


Fig.5. Growth of mean grain volume versus time for different particle volume fractions.

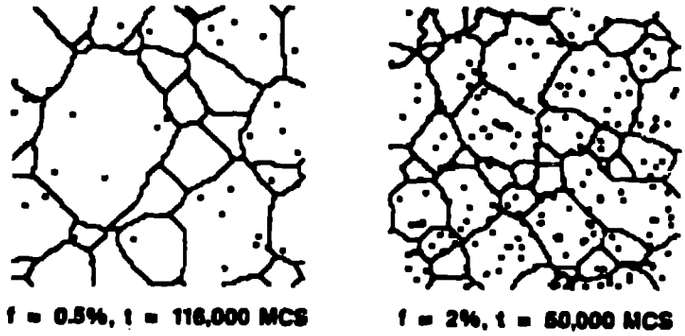


Fig.6. Pinned structures for two different particle fractions.

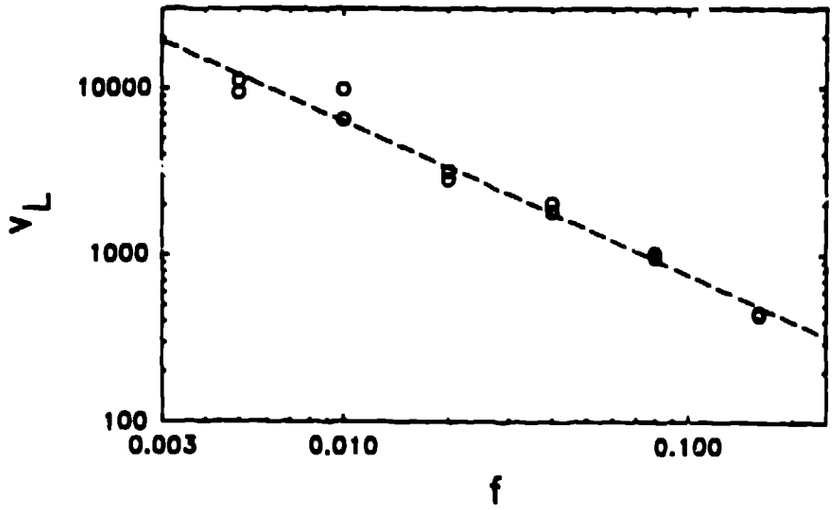


Fig.7. Limiting grain volume

This picture was partially confirmed by determination of the total fraction of particles on grain boundaries, ϕ, and the separate fractions of the particles on 2 grain faces, 3 grain edges and 4 grain corners, ϕ_2, ϕ_3 and ϕ_4 respectively. Fig.8 shows the observed values and it can be seen that they are much larger than would be expected for a random correlation of particles and boundaries. As discussed by Anderson et al.(1989b), the values of ϕ and ϕ_4 expected for a "Zener" situation of randon correlation of particles and boundaries are given by:

$$\phi(Z) = 3r/R_L \qquad (14)$$

and

$$\phi_4(Z) = 6r^3/R_L^3 \qquad (14a)$$

At $f = 0.01$, when $R_L/r = 18.2$, $\phi(Z) = 0.16$ and $\phi_4(Z) = 0.001$ compared to the measured values of $\phi = 0.41$ and $\phi_4 = 0.01$. The high meaured values of the fraction of particles on boundaries compared to the Zener values shows that in 3D, as in 2D, particle inhibited grain growth cannot, at least in the simulations, be treated by balancing the Zener drag on a boundary with the average driving force for grain growth, eq.7. A better structural model is required.

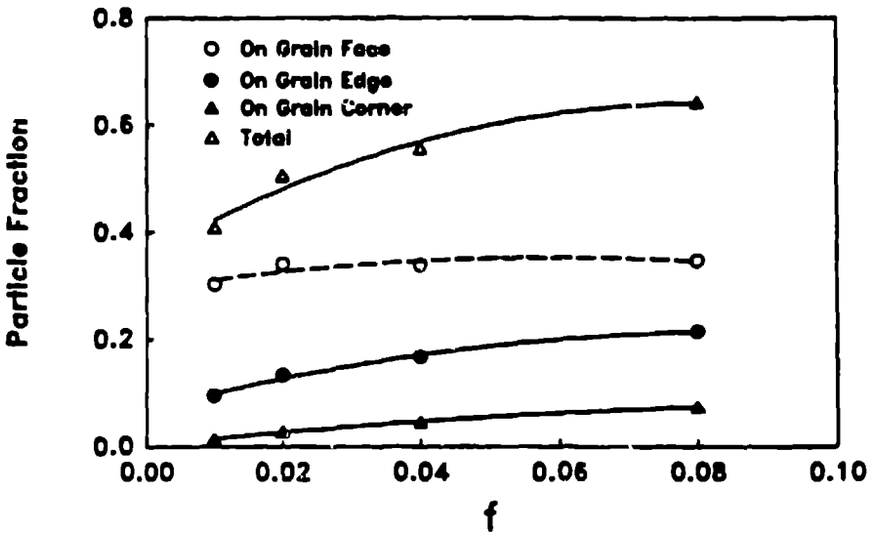


Fig.8 Fractions of the particles found at grain faces, ϕ_2, grain edges, ϕ_3, and grain corners, ϕ_4, and the total fraction of particles at boundaries, ϕ, in the pinned microstructures as a function of the volume fraction of particles, f.

In the 2D case Srolovitz et al. (1984b) and Hillert (1988) have argued that the pinning mechanism can be understood by the ability of particles to remove curvature, so that grains with less than six neighbours but in contact with particles will not disappear, see fig 4. This is easy to see in 2D structures but is much less transparent in 3D. Rhines and Craig(1974) in discussing the topology of grain growth, as revealed by serial sectioning an aluminium sample, found that the simplest small grains lay at the corners of 4 grain junctions and had the form of a tetrahedron, fig 9a. The requirement of 120° angles at grain edges and 109.5° angles at grain corners causes the convex shape shown - this curvature leads to the shrinkage and disappearance of such a grain. However if particles had pinned the 4 grain corners this will allow the grain edges to meet at particles at angles other than the required 109.5° angle. Under these circumstances the net curvature, $(1/R_1 + 1/R_2)$ could be reduced to zero by a balance of two opposite curvatures, fig 9b, thereby stabalizing such a grain against shrinkage.

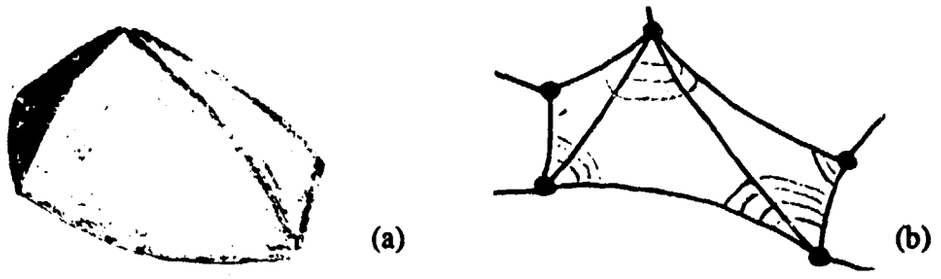


Fig. 9. (a) The convex shaped grain described by Rhines and Craig (1974) in single phase grain growth. (b) Possible similar sized grain pinned by particles at the grain corners showing zero net curvature.

In order to gain some further insight into this idea, the pinned grain structures in the 3D simulations are being studied in more detail to compare with the grain structures simulated in 3D single phase grain growth.

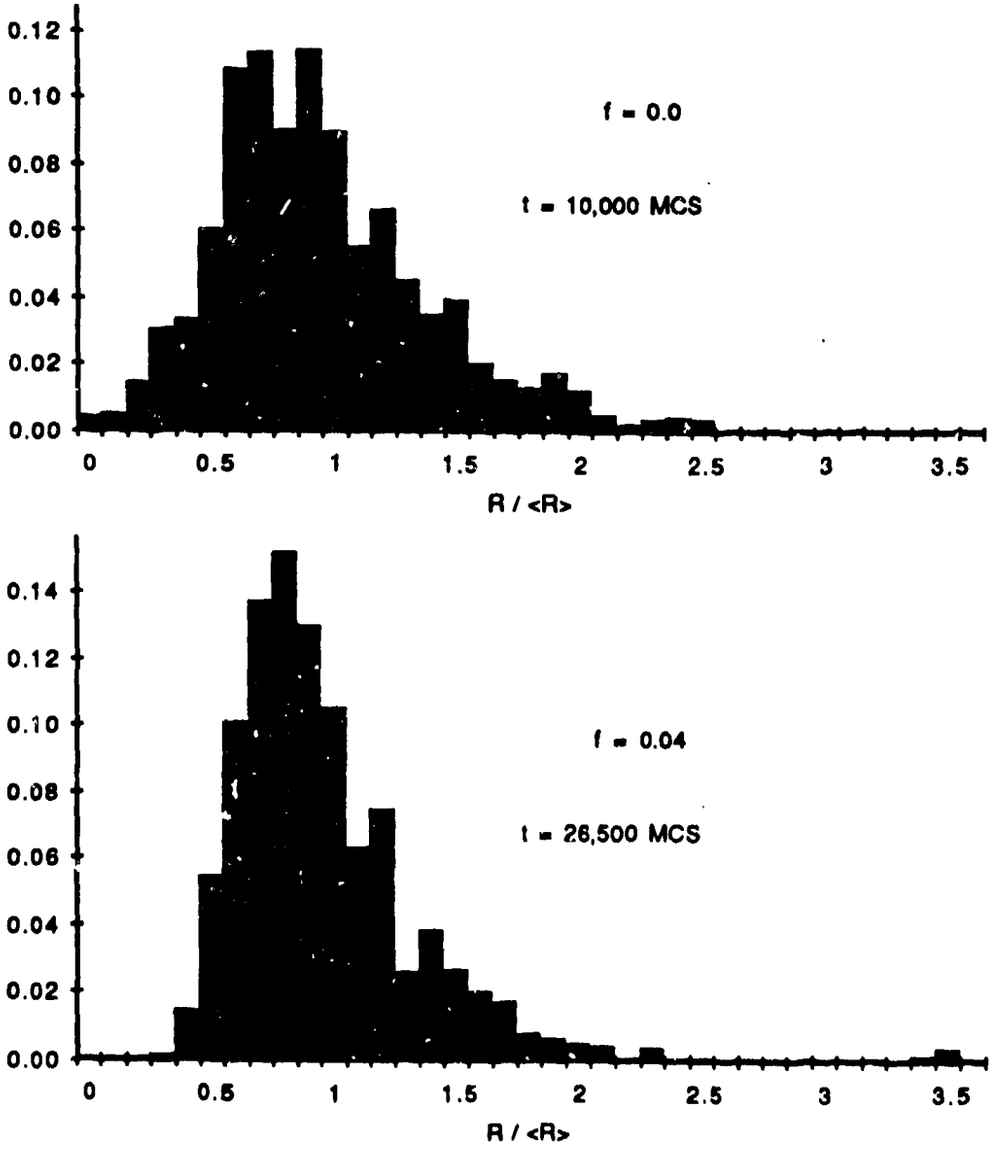


Fig.10. The measured grain size distribution in a single simulation for the single phase case, f =0, and for a pinned particle containing structure at comparable grain sizes.

Fig.10 shows the grain radii distributions, calculated from the "observed" grain volumes, for two microstructures, in fig 10a for the particle free case and in fig.10b for the pinned structure at f = 0.04. There is a significant statistical noise due to the limited number of grains (compare with fig 11e of Anderson et al. (1989a) for a statistically smoothed version of fig 10.a.). It is clearly seen (i) that the pinned structure is somewhat more sharply peaked with the peak of the distribution at values of R somewhat less than <R>, (ii) that there are markedly less very small grains in the pinned structure and (iii) that there is a suggestion of a very few much larger (abnormal) grains. The last observation is not yet clearly established but if it is confirmed it would be very significant in the light of the experimental observation of abnormal grain growth in low volume fraction particle containing material described later. The cut off at the small grain size has been firmly established in the results analysed so far. The physical significance of this cut -off seems to be that in the pinned structure all the smallest grains with R less than 0.3 <R> have already vanished while in the still dynamically evolving single phase structure these grains are in the act of vanishing but they will then be replaced by relatively larger grains that are in the next larger size classes. In the pinned grain structure the grains comparable to the smallest grains in the single phase structure have vanished - but they are not being replaced by the shrinkage of the next largest grains. This hypothesis gives the concept that normal grain growth ceases in the pinned structure when the smallest grains remaining in the distribution stop shrinking.

The other aspect of the pinned microstructures that has been very recently studied is the detailed topology of all grains with respect to their relative size, the distribution of particles at their boundaries, edges and corners and their numbers of adjacent matrix grains. Table 1 shows some initial results of this analysis for four of the microstructures.

Table 1. Analysis of computer simulated microstructure

	f = 0.0 <V> = 4,525	f* = 0.005 <V> = 11,111	f *= 0.01 <V> = 6,536	f *= 0.04 <V> = 1,938
Smallest 5% of grains	V/<V> = 0.03 N_N = 7.2	V/ <V> = 0.08 N_N = 8.1 n_3 = 4.2 n_4 = 0.9	V/ <V> = 0.06 N_N = 8.7 n_3 = 5.9 n_4 = 2	V/ <V=0.10 N_N = 9.1 n_3 = 12 n_4 = 9.5
Smallest 10% of grains	V/<V> = 0.04 N_N = 7.6	V/ <V> = 0.11 N_N = 8.5 n_3 = 4.7 n_4 = 1.1	V/ <V> = 0.08 N_N = 9.1 n_3 = 6.5 n_4 = 1.9	V/ <V> = 0.12 N_N = 9.2 n_3 = 13 n_4 = 9.2
Grains with V/ <V> = 0.12	N_N = 9.2	"	N_N = 10.3	"
45-55% of grain volume distribution	V/<V> = 1.0 N_N = 16.6	V/ <V> = 0.65 N_N = 13.6 n_3 = 12.2 n_4 = 2	V/ <V> = 0.50 N_N = 12.9 n_3 = 13.9 n_4 = 3.8	V/ <V> = 0.51 N_N = 12.6 n_3 = 31.2 n_4 = 12.5
Grains with V/ <V> = 1.0	"	62-71%of grains N_N = 16 n_3 = 13 n_4 = 2		72-74%of grains N_N = 16 n_3 = 43 n_4 = 16
Largest 5% of grains	V/<V> = 4 - 13	V/ <V> = 3 - 7	V/ <V> = 3 - 15	V/ <V> = 3 - 30

V/<V> is the mean of the ratio of the grain volume to the mean grain volume. N_N is the mean number of neighbouring grains. n_3 is the mean number of particles on grain edges. n_4 is the mean number of particles on grain corners. f* - pinned particle containing structure.

There are several striking points to be seen in table 1. The first is the variation in the size distribution between the particle containing and particle free structures previously noted in fig.10. The smallest grains seen in the single phase structure are missing from the pinned structure and the median value of the pinned distribution occurs at R less than <R> . The second feature of table 1 is the mean number of grain neighbours shared by the smallest grain size. This number is surprisingly large, with 7- 9 neighbours for all the microstructures. It might have been expected following a simple reading of the classic study by Rhines and Craig(1974) that most shrinking grains in a single phase structure would end their lives as tetrahedrons - this may in fact be the case but the probability of catching this transient form appears to be negligably small. It is however significant both for the single phase and particularly for the particle containing structures that the smallest grains are seen to be in contact with a large numbers of larger grains. Small grains have small faces - but these small faces are of course shared with the impinging large grains. The tension of the grain boundaries of these external grains, as they impinge on the smallest grains, will act to slow the shrinkage of the small grains. Another way of saying the same thing is to recognize that as the number of faces increases towards 14 the curvature causing shrinkage deceases, Rhines and Craig(1974). For the single phase case this structural feature will merely effect the kinetics of normal grain growth but for the particle containing structures, the ending of normal grain growth appears to take place by inability of the smallest grains to shrink away from the high density of particles and from the surrounding grain boundaries. The current conclusion from the early analysis of these structures is that in 3D, as in 2D, particles are very efficient at removing the net curvature of the boundaries - particularly at the smallest grains in the distribution. It is also apparent from table 1 that the pinned grain structures are not self-similar - there is a significantly higher concentration of particles at grain corners at the highest values of particle fraction, f. This higher concentration of particles corresponds to the smaller pinned grain size with high f, eq. 13, which have a larger driving force for shrinkage.

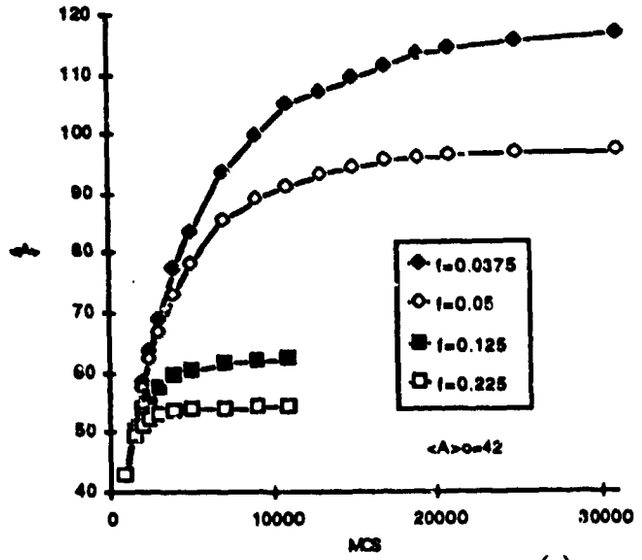
2D SIMULATION OF PARTICLE LIMITED GRAIN GROWTH FROM A FINITE GRAIN SIZE

This simulation was designed to model the micrstructural evolution in deformed metals grains which have recrystallized to a size determined by the relative rates of nucleation and growth in a deformed microstructure. The driving force for growth in recrystallization is usually much larger than the Zener drag, Ashby (1980), so at the end of recrystallization only random correlation of grain boundaries and particles would be expected, see Ashby et al.(1969). Grain growth will then continue from this structure expected to have a random correlation between particles and boundaries. This process is readily simulated - though results so far have been obtained only in 2D. The proceedure was to allow grain growth from the usual starting structure of a one lattice point grain size, Srolovitz et al.(1984a), to a mean grain area usually of 40 lattice points though some larger values were also used (80 and 160 lattice points). Having achieved these strarting structures with no particles, various area fractions of particles (0.0125 to 0.225) were randomly introduced into the structure and the simulation allowed to run. A full set of results with sufficient set of repeats to give improved statistics is not yet available but the initial results reported here clearly show the main trends. The values of starting grain size, $\langle A \rangle_0$, and area fraction, f, were chosen so that the Zener analysis would for some structures predict grain growth while at others with higher area fractions it should not be posible. The 2D version of eq.8 is:

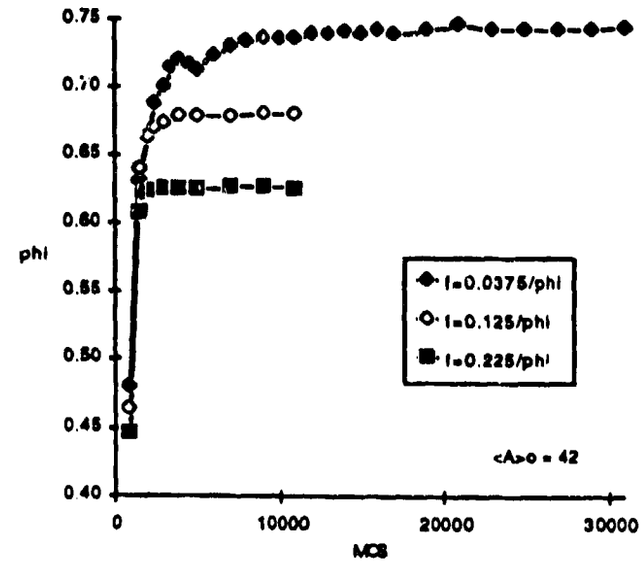
$$R = \pi r / 4 f \qquad (15)$$

$$A = \pi^2 a / 16 f^2 \qquad (15a)$$

At $\langle A \rangle_0 = 40$, eq.15b predicts no grain growth for $f > 0.124$. On the basis of previous simulations, and their reanalysis, Srolovitz et al.(1984b) and Doherty et al. (1987), it was expected that the values of the fraction of the particles on the boundaries and at the 3 grain edges, ϕ and ϕ_3, should increase from the random values at the start of the second stage simulation as grain boundaries migrated and became held-up at particles. It was, however, not known how quickly this might happen nor what the limiting grain sizes would be.



(a)



(b)

Fig. 11. Evolution of microstructure with time in MCS, from a starting grain area of 42, for several values of f. (a) The mean grain area and (b) the fraction of particles ϕ on the grain boundaries.

Fig.11a shows the growth in mean grain area while 11b shows that the increase in ϕ from a starting mean grain area $\langle A \rangle_0$ of 42 a. ϕ_3 increases at a compable way to ϕ. There is a steady increase in $\langle A \rangle$ owards a limiting valu. that takes longer to achieve at smaller values of f. The fraction of the particles generally on the boundaries and at 3 grain edges increased very much more rapidly to the limiting values. Fig. 12 shows the similar results using the larger starting grain sizes, but for the larger values of $\langle A \rangle_0$ only one volume fraction, f = 0.05, has so far been tested. The results are also given in tables 2-4 which also give details of the analysis of the results. Fig. 13 shows the limiting grain areas produced as a function of the reciprocal of f - together with the original results from Srolovitz et al. (1984b) for 2D particle limited grain growth from $\langle A \rangle_0 = 1$. For values of $f > 0.0375$, the simple result is produced:

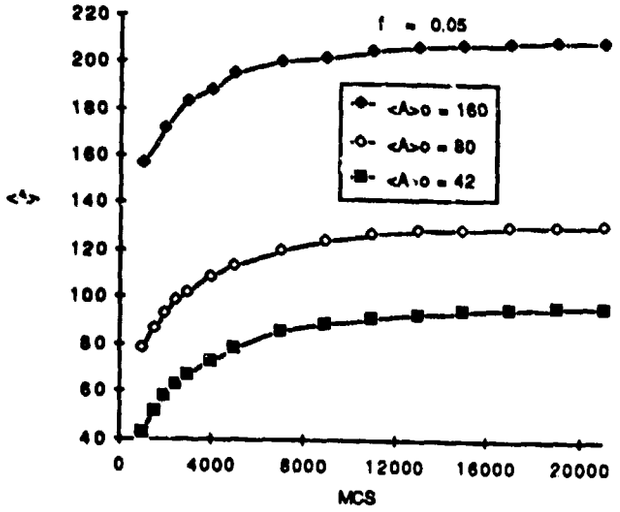
$$\langle A \rangle = \langle A \rangle_0 + 2.9 / f \qquad (16)$$

This is identical to that of Srolovitz et al.(1984b) for the f dependency but shows a striking increase in the limiting grain size directly arising from the larger starting grain areas. Initial results suggest that at larger values of 1/f the results are tending towards the original value, eq.11 or 16a.

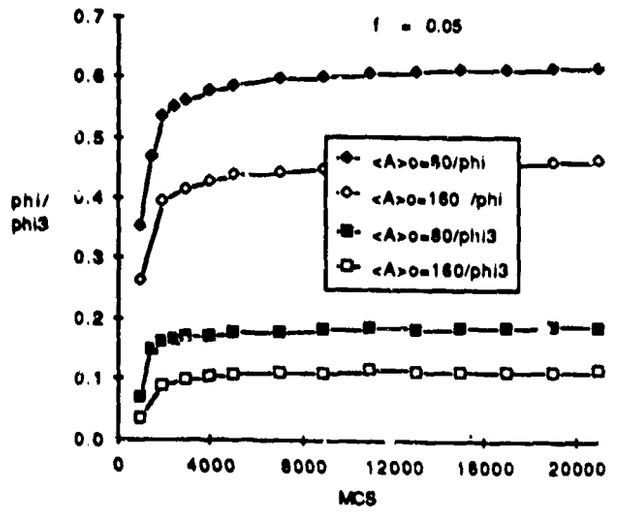
$$\langle A \rangle = 2.9 / f \qquad (16a)$$

As 1/f becomes larger the interparticle spacing, $(1/f)^{1/2}$ in 2D, becomes much larger than the starting grain size, $\langle A \rangle_0$, so it would be expected that the new results should merge with eq. 11a as f falls. However at small values of f longer times and more repeated runs are required to give statistically valid results for the pinned grain sizes. These will be published when available. The limiting values of ϕ and ϕ_3 as a function of 1/f (for $\langle A \rangle_0 = 42$) are shown in fig.14 (the largest value of 1/f shown in fig.14 is for a structure in which grain growth was still continuing though the ϕ values seem to have saturated. From fig.14 it can that, at small values of 1/f, the values of ϕ are smaller than those found for $\langle A \rangle_0 = 1$. With $\langle A \rangle_0 = 1$, ϕ fell from 0.9 at 1/f = 20 to 0.86 at 1/f =100 and to 0.8 at 1/f = 200, Srolovitz et al (1984b). Both the limiting

values of <A> and ϕ are functions of $\langle A \rangle_o$ and f, unless $\langle A \rangle_o$ is very much less than $(1/f)^{1/2}$.



(a)



(b)

Fig.12. Evolution of microstructure at f = 0.05, from different starting grain sizes. (a) the mean grain area and (b) the fraction of particles generally at boundaries ϕ and at 3 grain corners ϕ_3.

For 2D hexagonal grains in a hexagonal lattice the simple result that a hexagon of side h will cover A lattice points such that:

$$A = 3h^2 - 3h + 1 \qquad (17)$$

This is readily derived - for example by determining the area as the sum of the number of lattice points in 3 rhomi of sides h by h (h^2), less the sites double counted in 3 rows of length h (-3h) that meet at the center site that needs then to be included (+1). For A > 1 this yields

$$h = \{3 + (12A - 3)^{1/2}\} / 6 \qquad (17a)$$

Inspection revea that there are (12h - 6) lattice points adjacent to the boundaries of such a hexagonal grain. 18 of these boundary point are associated with the 6 triple points, each shared with 3 grains, so each triple point contributes 6 sites per grain. The remaining (12h - 24) sites are each associated with boundaries between 2 grains, so these sites contribute a further (6h - 12) boundary sites to each grain. This gives a total of (6h - 6) boundary sites for each h sided grain. The fraction of sites in contact with grain boundaries F(b) is then the the product of (6h - 6) sites per grain with the number of grains N_G divided by the number of lattice points N_P. But $N_G / N_P = 1 / \langle A \rangle$.

$$F(b) = (6h - 6) / \langle A \rangle \qquad (18)$$

For a Zener-like random correlation of particles with grain boundaries we then obtain after substituting <A> for A in eq.17a:

$$\phi(z) = F(b) = \{ (12 \langle A \rangle - 3)^{1/2} - 3 \} / \langle A \rangle \qquad (19)$$

The fraction of particles at 3 grain triple point in the random structure is readily estimated as follows. Each hexagonal grain has 6 triple points each sourrounded by 3 lattice points giving

18 points but these are shared between 3 grains so giving 6 lattice "triple" points per grain. This immediately yields, for a random correlation of particles and grain boundaries:

$$\phi_3(z) = 6 / \langle A \rangle \qquad (20)$$

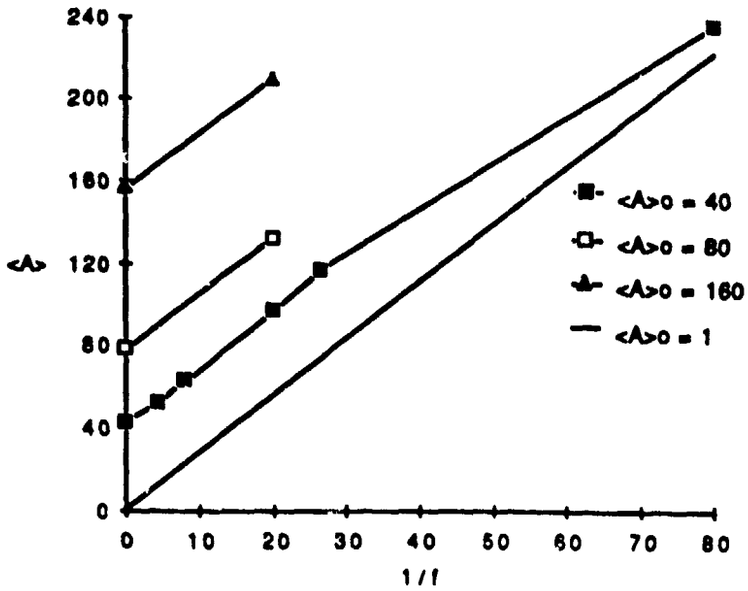


Fig.13. The limiting grain areas as a function of 1/f and the starting grain area, $\langle A \rangle_0$.

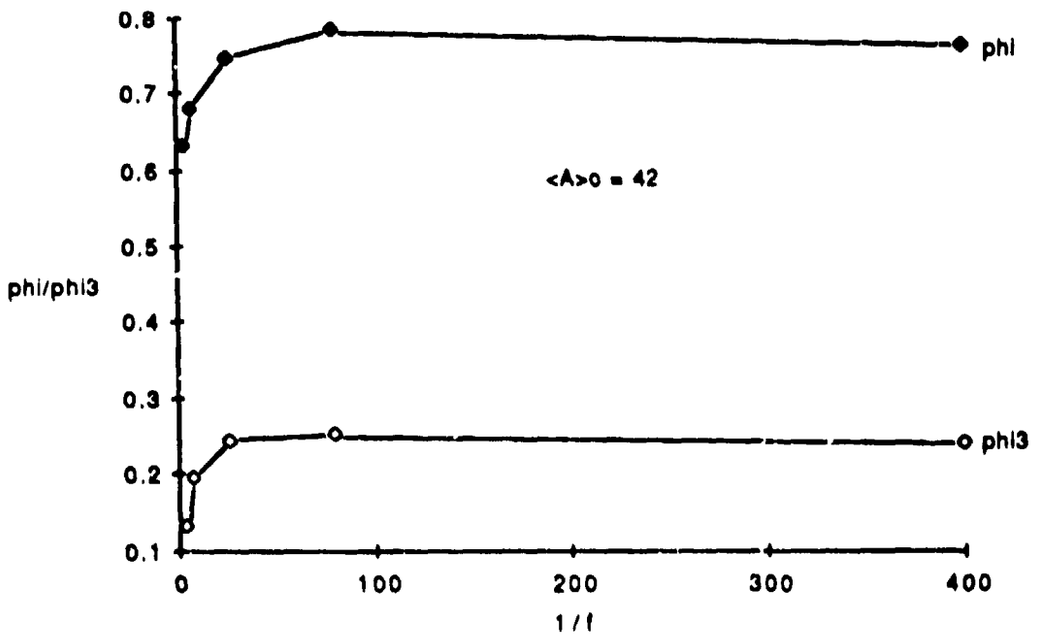


Fig.14. The limiting values of the fraction of particles on grain boundaries, ϕ, and the fraction on 3 grain corners, ϕ_3, as a function of 1/f for $\langle A \rangle_0 = 42$.

Table 2 gives details of the initial starting structures and shows that eq. 19 gives close agreement with the observed values of ϕ, however eq. 20 slightly overestimates the values of ϕ_3. Table 3 shows the details of the pinned structures and the predicted values of $\langle A \rangle(z)$, $\phi(z)$ and $\phi_3(z)$ predicted for a random correlation of boundaries and particles.

Table 2. Initial 2D Simulation Microstructure

$\langle A \rangle_o$	f	ϕ	ϕ_3	$\phi(z)$	$\phi_3(z)$
42.8	0.0125	0.48	0.10	0.46	0.14
42.6	0.0375	0.48	0.12	0.46	0.14
42.6	0.1250	0.47	0.12	0.46	0.14
42.9	0.2250	0.45	0.10	0.46	0.14
77.8	0.0500	0.35	0.07	0.35	0.077
157	0.0500	0.26	0.034	0.26	0.038

Table 3. Pinned 2D Simulation Microstructure

$\langle A \rangle_o$	f	$\langle A \rangle$	$\langle A \rangle(z)$	ϕ	ϕ_3	$\phi(z)$	$\phi_3(z)$
42.8	0.0125	235	3940	0.78	0.25	0.21	0.025
42.6	0.0375	117	438	0.74	0.24	0.29	0.051
42.5	0.0500	97.1	246	0.72	0.26	0.32	0.062
42.6	0.1250	62.3	39.5	0.68	0.20	0.39	0.096
42.9	0.2250	54.0	12.2	0.63	0.13	0.41	0.110
77.8	0.0500	131.5	246	0.62	0.19	0.28	0.046
157	0.0500	209.4	246	0.46	0.115	0.23	0.029

During growth there is a rapid initial increase in the values of ϕ and ϕ_3. But the expected random or Zener values, eqs. 19 and 20, predict a fall as the mean grain size grows. That is there is during the intial period of grain growth a rapid evolution in the correlation of particles and boundaries and triple points as the boundaries move to particles and are held there - this of course leads to a slowing in the rate of grain growth - which on an A /MCS (time) plot would be linear if no particle inhibition of motion were present, Anderson et al. (1984). Somewhat surprisingly, the values of ϕ and ϕ_3 saturate much sooner than does $\langle A \rangle$, that is grains are still disappearing even though there is no further increase in the particle / boundary correlation. A similar effect, though perhaps a less obvious feature, can be noted in the original 2D particle simulations of Sorolvitz et al.(1984b). Two processes seem to be occuring in the present study. First there is a short period of time in which the fraction of particles on the boundaries increases while general grain growth is occuring. Thereafter there is no further increase in the fraction of particles on the boundaries but the mean grain size continues to increase - indicating that smallest grains, not in contact with particles, are still disappearing. Small grains not in contact with more than 2 particles should be able to vanish, fig.4. This idea can be explored further by use of the grain size distribution in the 2D single phase simulations, fig. 10 of Srolovitz et al (1984a). Table 4 shows the fraction of grains, G_d, that have disappeared as the grain size grew from the original value, $\langle A \rangle_o$, to the final value $\langle A \rangle$ seen in table 3, α is the grain size ratio, $R^*/\langle R \rangle_o$, with R^* and A^* the radii and areas of the smallest class of grains present at the start of grain growth that survives the period of particle limited grain growth and P^* is the mean number of particles in contact with or inside these critical sized grains which were all treated as though hexagonal. P^* appears to be close to the critical value of 3 - apart that is from the extreme values of f. This failure at small f is not surprising since at the large values of 1/f the critical sized grains that just survive will first grow to the interparticle spacing, $(1/f)^{1/2}$, so increasing the number of particles that they contact before they try to shrink back. The increase in P^* at large f is not however understood and may indicate that the current analysis is flawed in some way.

A final point is worth making about the data shown in table 3. The Zener model seems to fail in two opposite ways. At small volume fractions it underestimates the magnitude of the particle inhibition of grain growth just as in the earlier simulations - more significantly however it also fails when a large initial grain size is produced and given a high density of randomly distributed

particles. The Zener analysis predicts that there should be no grain growth - but growth is seen. This arises since many small grains do not contain a critical number of particles to stop their collapse, giving a significant decease in the number of remaining grains.

Table 4. Grain Growth Analysis

$\langle A \rangle_o$	f	$\langle A \rangle$	Gd	α	A*	P*
42.8	0.0125	235	0.82	1.06	48	1.0
42.6	0.0375	117	0.64	0.97	39.5	2.5
42.5	0.0500	97.1	0.56	0.86	31.5	2.8
42.6	0.1250	62.3	0.32	0.57	13.8	4.1
42.6	0.2250	54.0	0.21	0.47	9.6	5.8
77.8	0.0500	131.5	0.41	0.65	59.1	3.0
157	0.0500	209.4	0.25	0.52	70.8	3.5

In conclusion, both series of simulation studies show that the Zener analysis based on random particle boundary correlation fails and an alternative model is required. The current results suggests that a more successful model will be one based on the effect of particles on removing the curvature required for grain growth. During growth from a very small grain it can be seen that grains grow until the grain size is comparable to the interparticle spacing, $(1/f)^{1/2}$ in 2D and $(1/f)^{1/3}$ in 3D. During growth from a finite grain size comparable to or larger than the interparticle spacing the current results suggest that those grains that contain less than a critical number of particles about 3 in 2D will vanish. Further simulations will be required to study the important problem of 3D growth from a finite grain size.

5. EXPERIMENTAL STUDIES IN Al-Fe

In order to provide some verification of the validity of the computer models some brief experiments have been carried out using an Al - 0.15wt% Fe - 0.07% Si alloy supplied by Alcoa for a different research project. This alloy, after casting and high temperature homogenization has a low volume fraction, f = 0.002, dispersion of coarse Al_3Fe particles that are very stable during long high temperature anneals. Such a system is ideally suited to distinguish between eqs 8 and 13. The as-cast material has been shown to have a near random texture and was homogenized at 620°C for 24 hrs and heat treated at 450°C for 72 hours to precipitate a fine dispersion of the cubic AlFeSi phase. Samples were then cold rolled 20, 30, 34, 40 or 60% and recrystallized at temperatures between 500°C (20 and 30% deformation) to 400°C (60%) for 4 hours. At these lower temperatures the AlFeSi phase pins grain growth so the as recrystallized grain size could be readily determined. The materials were then placed in an air furnace at 620°C and held for various lengths of time - shown in table 5. Conductivity and SEM studies showed that the fine AlFeSi phase dissolved up completely in less than 1 hour at 620°C. The grain size was determined by the linear intercept method and the results shown in table 5. An unexpected complication of this study was the ready intervention of abnormal grain growth giving isolated huge grains whose size was frequently limited only by the specimen dimensions. This occured for materials rolled more that 34% giving as recrystallized grain sizes of 130 microns or less. However even with abnormal grain growth it was sometimes possible to find a region of the sample showing a sufficient number of matrix grains for the grain size of these matrix grains to be determined.

For the mean size of particles, $\langle r \rangle = 2\mu m$ the Zener analysis predicts a pinned grain size of $1300\mu m$ - very much larger than the limiting grain size seen of $200\mu m$. The 3D computer simulation starting at a very fine grain size predicts $62\mu m$ - 3 times smaller than seen but no correction can be made for the finite grain size effect since this has not yet simulated in 3D.

Qualitatively this effect is expected to increase the predicted value of the final grain size but the magnitude of the increase is at present unknown. Attempts to avoid this difficulty by reducing the grain size produced the abnormal grain growth effect seen.

Table 5. Observed grain sizes (in μm) after different times at 620°C

Reduction	Rex.Temp	As-Rexed	1hr	4hr	8hr	20hr	112hr
20%	500°C	280	254	274	-	270	272
30%	500°C	176	186	-	-	208	-
34%	450°C	200	208	-	-	220	-
40%	450°C	132	208	234	A	A	-
60%	400°C	85	200	A 215	A 192	A 208	-

A - indicates that abnormal grain growth has occured in part or most of the sample.

The obvious first question about this abnormal grain growth is why might it have occcured? Brief texture studies have shown that the as-recrystallized material has a very weak texture and the abnormal grains appear to have no special orientation with respect to the rolling geometry. The brief review of the physics of particle drag at the start of this paper immediately suggests, however, an attractive hypothesis. The Zener analysis leading to eq. 8, while not appropriate for normal grain growth, should remain valid for abnormal grain growth. This process occurs by migration of the boundaries of a few, very large grains. For abnormal grain growth, <D> in eq.8 will be the maximum matrix grain size that should just support the growth of an abnormal grain that was very much larger than the pinned matrix grain size. The pressure balance leading to eq. 8 is precisely that required for just preventing abnormal grain growth provided a large grain has developed. So abnormal grain growth can, on this basis, be predicted to be possible whenever the matrix grain size is pinned by particle inhibited normal grain growth (eq. 13 as modified by finite starting size effect) and when a very large grain is present. The current data suggests that with starting grain sizes less than 140μm, the required nucleation of abnormal grain growth can take place. Initial further experiments that support this have been carried out by attempting to provide such a nucleus by a localized hardness indentation. So far this has only been carried out on as-cast material (with a starting grain size of 150μm). This material without indentations usually resists abnormal grain growth except for anneals of 1 week or more - but it always shows abnormal grain growth from indentations after a few hours at 620°C. These tentative conclusions from this, so far very limited data, clearly need confirmation by further experiments - but if these ideas are confirmed they could be of very major significance in understanding the conditions for this usually undesirable process. Limited support is provided by the observation by Calvet and Renon(1960) of abnormal grain growth in deformed aluminium alloys when annealed at each alloy's solvus temperature (that is where f -> 0). It is an obvious question as to why, if this idea is true, that our 3D simulations did not show this effect. Some limited indication of the possibility of abnormal grain growth was briefly described in the studies of precipitate size distributions, see also fig.6. There is an interesting but frustrating limitation on the 3D simulations - at small volume fractions the matrix grains are becoming comparable to the array size giving both very long runs and very limited numbers of grains that might act as potential nuclei. Experiments with inserted large grain nuclei in pinned 3D are therefor clearly required and are under way. Such experiments of course failed to give abnormal grain growth in 2D, Srolovitz et al.(1985), but given the curvature inhibiting effect of particles in 2D that failure is of course now expected.

6. CONCLUSIONS

The 3D simulations show that the limiting grain size following normal grain growth from a small grain size is a simple function of $(1/f)^{1/3}$ - with a much higher than random corelation of

particles with grain boundaries. The pinned grains had a small grain size cut-off at a higher fraction of the mean grain size than is seen in the single phase simulations. 2D simulations from a finite grain size showed that the limiting grain size is a strong function of both the starting grain size as well as the particle fraction. These simulation results show that the Zener model is seriously flawed for normal grain growth for which a better model is one based on the ability of particles, in both 2D and 3D, to remove boundary curvature. Limited experimental results has been obtained and these support these conclusions but show, at small as recrystallized grain sizes and low volume fractions of particles, a ready transition to abnormal grain growth. Such a transition can be readily understood on the basis that the Zener limit though failing for normal grain growth is a valid model for predicting the limiting grain size that will allow the growth of a few large grains. Further experiments and more simulations are required to confirm these initial results.

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