Acta metall. Vol. 37, No. 2, pp. 627–639, 1989
Printed in Great Britain.

0001-6160/89 $3.00 + 0.00

COMPUTER SIMULATION OF RECRYSTALLIZATION IN NON-UNIFORMLY DEFORMED METALS

A. D. ROLLETT,[1] D. J. SROLOVITZ,[2] R. D. DOHERTY[3] and M. P. ANDERSON[4]

[1]Los Alamos National Laboratory, Los Alamos, NM 87545, [2]University of Michigan, Ann Arbor, MI 48109, [3]Drexel University, Philadelphia, PA 19104 and [4]Exxon Research and Engineering Co., Annandale, NJ 08801, U.S.A.

(*Received* 20 *April* 1988)

Abstract—The classical Johnson–Mehl–Avrami–Kolmogorov (JMAK) equation $[F = 1 - \exp(-kt)^n]$ for nucleation and growth transformations works very well for most solid state transformations but fails regularly when applied to recrystallization of plastically deformed metals. Under conditions of near constant growth rate, a high exponent ($n \geqslant 3$) is predicted but low exponents ($n \leqslant 2$) are typically measured. Another common observation is that the slope of a JMAK plot, from which the exponent is inferred, decreases as recrystallization proceeds. Analysis of the published data suggested the hypothesis that the failure of the JMAK theory as applied to recrystallization is because of the lack of uniformity of the stored energy of plastic deformation on the grain size scale. This hypothesis was tested by use of Monte Carlo simulations of the type previously used successfully to model grain growth and recrystallization. The earlier simulations of recrystallization used uniform stored energies whereas the simulations presented here varied the stored energy from grain to grain. The kinetics were plotted on JMAK plots which exhibited low and varying exponents closely resembling experimental data. Specific simulations were performed to test the basic JMAK assumption that makes a correction for the effect of impingement under conditions of random nucleation, namely $dF/dF_e = (1 - F)$, where F is the actual volume fraction and F_e is the extended volume fraction—that which would obtain in the absence of impingement and overlap between new grains. It was found the assumption is accurate under conditions of uniform stored energy. With non-uniform stored energy, however, the correction underestimated the effect of impingement by a factor that rapidly increased (to over two orders of magnitude) during recrystallization.

Résumé—L'équation classique de Johnson, Mehl, Avrami et Kolmogorov (JMAK), $[F = 1 - \exp(-kt)^n]$, pour les transformations par germination et croissance conveient très bien pour la plupart des transformations de l'état solide, mais elle échoue régulièrement quand on l'applique à la recristallisation des métaux déformés plastiquement. Dans des conditions de vitesse de croissance à peu près constante, elle prédit un exposant élevé ($n \geqslant 3$) alors que l'on observe typiquement des valeurs basses ($n \leqslant 2$). On observe aussi couramment que la pente d'une courbe JMAK, a partir de laquelle on détermine l'exposant, décroît au course de la recristallisation. Une analyse des résultats publiés laisse penser que la raison de l'échec de la théorie JMAK, lorsqu'on l'applique à la recristallisation, est le manque d'uniformité, à l'échelle du grain, de l'énergie de déformation plastique emmagasinée. Nous avons testé cette hypothèse à l'aide de simulations de Monte Carlo du même type que celles qui avaient été utilisées précédemment avec succès pour modéliser la croissance des grains et la recristallisation. Les premières simulations de recristallisation utilisaient des énergies emmagasinées uniformes, alors que les simulations que nous présentons dans cet article font varier l'énergie emmagasinée d'un grain à l'autre. La cinétique évolue selon des courbes JMAK dont les exposants, peu élevés et variables, correspondent bien aux résultats expérimentaux. Nous avons réalisé des simulations spécifiques pour vérifier si l'hypothèse JMAK de base corrige l'effet de rencontre des grains dans des conditions de germination aléatoire, c'est-à-dire si $dF/dF_e = (1 - F)$, où F est la fraction volumique réelle et F_e la fraction volumique au sens large, c'est-à-dire celle que l'on obtiendrait en l'absence de rencontre et de chevauchement de nouveaux grains. L'hypothèse est exacte dans des conditions d'énergie emmagasinée uniforme. Cependant, pour une énergie emmagasinée non uniforme, la correction sous-estime l'effet de la rencontre des grains d'un facteur qui augmente rapidement (jusqu'à plus de deux ordres de grandeur) pendant la recristallisation.

Zusammenfassung—Die klassische Johnson–Mehl-Avrami-Kolgomorov-Gleichung (JMAK) $[F = 1 - \exp(-kt)^n]$ für Keimbildungs- und Wachstumsumwandlungen beschreibt die meisten Festkörperumwandlung sehr gut, ist aber regelmäßig fehlerhaft, wenn sie auf die Rekristallisation von plastisch verformten Metallen angewendet werden soll. Unter Bedingungen nahezu konstanter Wachstumsraten wird ein hoher Exponent ($n \geqslant 3$) vorausgesagt, aber kleine ($n \leqslant 2$) werden immer gemessen. Eine andere allgemeine Beobachtung betrifft die Steigung in der JMAK-Auftragung, aus der der Exponent folgt; diese Steigung nimmt mit vorwärtsschreitender Rekristallisation ab. Eine Analyse der veröffentlichten Daten legt nahe, daß diese Fehlerhaftigkeit der JMAK-Theorie aus der ungleichen Verteilung der gespeicherten Energie in den Körnern folgt. Diese Hypothese wurde mit Monte-Carlo-Simulationen der Art, wie früher erfolgreich für das Modell des Kornwachstums und der Rekristallisation benutzt, geprüft. Die früheren Simulationen der Rekristallisation benutzten gleichmäßig gespeicherte Energien, wohingegen die hier vorgelegten unterschiedliche gespeicherte Energien in den einzelnen Körnern berücksichtigen. Die in den JMAK-Diagrammen sichtbare Kinetik zeigte niedrige und unterschiedliche Exponenten, welche den experimentellen Ergebnissen ähnelten. Spezielle Simulationen wurden durchgeführt, um die Grundannahme der

JMAK-Gleichung zu prüfen, mit der eine Korrektur des Einflusses durch aufeinanderstoßende Körner bei statistischer Keimbildung durchgeführt wird, nämlich $dF/dF_e = (1 - F)$; hier ist F der aktuelle Volumanteil, F_e der erweiterte Volumanteil, also derjenige, der sich bei Abwesenheit des Aufeinanderstoßens und des Überlappens von Körnern ergäbe. Es ergibt sich, daß diese Annahme bei gleichmäßig gespeicherter Energie richtig idst. Ist diese jedoch ungleichmäßig, dann unterschätzt die Korrektur den Einfluß des Aufeinanderstoßen um einen Faktor, der rasch während der Rekristallisation auf über zwei Größenorndungen ansteight.

1. INTRODUCTION

Recrystallization is a process of fundamental importance in the thermomechanical processing of metals since, in general, it restores a worked metal to an unworked and formable state. Primary recrystallization usually occurs by a discontinuous reaction where high angle grain boundaries sweep through a highly dislocated matrix, leaving behind material with a low dislocation density. It has frequently been observed that this reaction commences from a limited number of points or nuclei whose density is a strong function of the amount of strain accumulated in the material.

Several theories have been proposed to describe recrystallization kinetics. The most widely used theory for recrystallization and other nucleation and growth reactions is that developed independently by Avrami [4–6], Johnson and Mehl [7], and Kolmogorov [8] (JMAK). Kolmogorov's work has not received significant attention in the Western literature but it deserves to be put on an equal footing with the latter authors.

This type of theory assumes that the nucleation sites are randomly distributed in space. The true volume fraction of recrystallized material, F, can be estimated from the "extended volume fraction", F_e, which is the volume fraction that the new grains would occupy in the absence of impingement and overlap of adjacent recrystallized grains. Provided that the JMAK assumption of random nucleation holds, the relationship between F and F_e [5, 7] is obtained from

$$dF = (1 - F)\, dF_e. \tag{1}$$

If all nucleation events occur at time zero with a density I (number/unit volume) and isotropic growth occurs at a constant rate in three dimensions, G

$$dF_e = 4\pi I G^3 t^2\, dt. \tag{2}$$

Integration of equations (1) and (2) yields

$$F = 1 - \exp(-F_e) = 1 - \exp - (4/3\pi I G^3 t^3). \tag{3}$$

For other simple power law relationships for nucleation and growth rates, equations similar to equation (3) are obtained, see for example Christian [3] and Cahn [9]. The general equation, often referred to as the JMAK equation, is

$$F = 1 - \exp(-kt^n). \tag{4}$$

The parameters of the equation are the kinetic parameter, k [$=4/3\pi IG^3$, in equation (3)] and an exponent, n. The exponent, n, is referred to as the JMAK exponent.

The focus of this paper is the JMAK exponent which is the most commonly used measure of recrystallization kinetics in experimental studies. Failure of the fundamental assumption of the JMAK theory as expressed in equation (1) is shown below to cause significant deviation from the theoretically expected values of the exponent. This deviation is almost universally observed in recrystallization experiments. The usual experimental determination of n is made by plotting equation (4) in a double logarithmic form and taking n to be the slope

$$\log[-\ln(1 - F)] = \log(k) + n \log(t). \tag{5}$$

Such a plot, usually referred to as a Johnson–Mehl–Avrami or JMAK plot, is commonly used to determine the kinetics of the transformation under study. The magnitude of the exponent can be shown theoretically to be closely linked to the morphology of nucleation and growth [3, 9]. Specifically, if growth takes place isotropically in three dimensions and all nuclei are present at time zero, the value of the exponent is predicted to be three. A reaction in which all nuclei are present at the beginning of the reaction will be referred to as "site saturated". If three dimensional growth occurs but nuclei appear at a constant rate in the unrecrystallized material, which will be referred to as the "continuous nucleation" condition, the value of the exponent is predicted to be four. Lower values of n are predicted for such conditions as growth in less than three dimensions and heterogeneous nucleation on planar or linear defects [3, 9]. In many experimental studies, however, low values of the exponent have been found without convincing evidence for nucleation being limited to defects of less than three dimensions [10].

Historically, the most important verification of the JMAK theory was perhaps the much quoted paper by Anderson and Mehl [11]. They measured rates of nucleation and growth in a lightly deformed fine grained sheet of aluminum. The growth rate, G, was effectively constant, though only in two dimensions in the thin sheet. The nucleation rate, I, varied exponentially with time but the authors were able to use equation (1) to derive a kinetic equation, similar to equation (4), that successfully linked the measured values of I and G to the overall recrystallization kinetics. This then provided support for the validity of equation (1).

The significant feature of Anderson and Mehl's microstructure [11] is that the recrystallized grains are much larger than the deformed, unrecrystallized grains. The sites for nucleation at small strains are almost certainly pre-existing grain boundaries [12]. Taking these two facts together suggests that only a small fraction of the possible nucleation sites actually operate. Under these conditions the spatial distribution of nucleation sites is effectively random [9], as required by equation (1). Gordon [13] used similar conditions in his studies of recrystallization of copper and obtained reasonable JMAK exponents of approximately 4. Apart from these two studies and the special case of Galibois and Dube [14], discussed below, almost all other studies of recrystallization kinetics have found unacceptably low values of the JMAK exponent.

The vast majority of experimental studies have shown exponents that were less than two, without microstructural evidence that the growth morphology was other than three dimensional or that there was a special nucleation morphology. A specific example is the study of Michalak and Hibbard [15] on the recrystallization of rolled, very low carbon steel, a material very similar to that used by Galibois and Dube [14]. They found exponents between 0.5 and 1.2, which were very much lower than the values of 2.4–4.3 determined by Galibois and Dube. Many other studies in Al, Cu and Fe have also found low exponents (see for example Rosen *et al.* [16], Perryman [17], Faivre [18], Fricke and McShane [10], Juul Jensen [19], Compte and Form [20], Petkovic *et al.* [21], Luton *et al.* [22], and Hansen *et al.* [23]). The articles by Setzer and Morris [24] and Laurent and Batisse [25] reviewed a number of previous studies that had reported low exponents.

The study of recrystallization in ultra low carbon steel by Galibois and Dube [14] showed exponents in the theoretically expected range for random nucleation and three dimensional growth, 2.4–4.3. The special feature of this study, however, was that a high stored energy was induced in their material not by plastic deformation but by quenching from the austenite phase. The quench produced a heavily dislocated lath martensite whose dislocation substructure is expected to be uniform. This uniformity of dislocation density is in contrast to the orientation dependence (on the grain scale) expected and observed for plastic deformation (see for example Kallend and Huang [26]). This dependence of stored energy as a function of crystallographic orientation is discussed below in more detail.

An important experimental observation of recrystallization that has been made on many occasions, but not properly quantified, is that the distribution of recrystallization nuclei is heterogeneous. Observations have been made of grains or regions of a deformed metal that are difficult (or slow) to recrystallize. For example, Carmichael *et al.* [27], Rosen *et al.* [16] and Inokuti and Doherty [28] have observed grains in a deformed metal that are either entirely lacking in nuclei or have far fewer nuclei than their neighbors. Figure 1, shows the microstructure of rolled copper that has been partially recrystallized where it is clear that the nucleation density varies markedly from one location to another in the deformed microstructure. Such nucleation heterogeneities can sometimes be associated with specific structural features. Adcock [29], in his classic work on rolled Ni–Cu alloys, showed how nuclei can arise on shear bands (i.e. regions of intense local deformation). Embury *et al.* [30] are currently studying the recrystallization of Al–Mg alloys (which form copious shear bands in rolling) in an effort to quantify the kinetics of this type of nucleation. Particle stimulated nucleation, PSN, is an obviously heterogeneous nucleation mechanism. Nes and Solberg [31] found that particles, in commercial purity aluminum, led to clusters of nuclei with random orientations. Away from these clusters, however, cube-oriented nuclei could be found.

It is of interest to note that in studies of nucleation and growth kinetics in structural transformations other than recrystallization, the expected values of the JMAK exponent are found. Examples include Christian's report of isothermal studies of an allotropic transformation in Mn [3] and, more recently, isothermal studies of polymorphic reactions in metallic glasses by Ahktar [32]. In both these examples linear JMAK plots were obtained with exponents of nearly 4. In diffusion controlled precipitation reactions studied by Servi and Turnbull [33] in Cu-Co alloys, exponents of 1.5 ± 0.5 were found. These JMAK exponents are compatible with site saturation nucleation conditions and diffusion limited growth where the particle radius is proportional to the square root of time. Fine [34] used data for the precipitation of carbon in α-iron from Wert and Zener [35] to show that the exponent is only approximately 1.5 for this case because the JMAK correction, equation (1), is not accurate for diffusional reactions with "soft impingement" of the solute fields between neighboring precipitates. This is in contrast to the "hard impingement" that occurs between recrystallized grains, new grains in polymorphic transformations or, for example, in eutectoid decomposition.

It is commonly observed that nucleation of recrystallization occurs at grain boundaries [36] and since Cahn's analysis [9] has given a low exponent for site saturated grain boundary nucleated reactions, it might be felt that this provides an explanation for the low recrystallization exponents. This is clearly mistaken, however, since site saturated nucleation on grain boundaries means that all grain boundaries will be coated with new grains. This is observed in eutectoid decomposition [37], for example, but almost never in recrystallization (see Fig. 1).

One possible explanation for lowered exponents is the simultaneous occurrence of recovery that reduces the driving force for recrystallization. Vandermeer

Fig. 1. Microstructure of copper uniaxially compressed 179% and partially recrystallized by annealing for 3 h at 200°C, showing nonhomogeneous distribution of recrystallized grains. Image obtained under channeling contrast conditions in a scanning electron microscope.

and Gordon [36] used this explanation in their study of alloys of aluminum with small amounts of copper. Their study showed that the growth rate of new grains decreased with time. Several other studies, however, have shown that prior recovery treatments have little effect on recrystallization kinetics (e.g. Laurent and Batisse [25], Rosen *et al.* [16] and Perryman [38]). Fig. 2 is taken from Rosen *et al.*'s study of recrystallization in iron and shows JMAK plots of the recrystallization kinetics at two different temperatures. At each temperature, the material was given various recovery treatments prior to recrystallization with very little effect. This same figure also exhibits low exponents: one at short times and much less than one at long times. Perryman [38] also obtained low exponents of 1.4–1.43 but he showed for his material that the nucleation rate and growth rates were constant during all but the first few percent of recrystallization. The effect of recovery should be to cause the growth rate to decrease continuously during recrystallization. Therefore recovery seems not to be a plausible explanation of the low exponents found in many studies of recrystallization.

The conclusion to be drawn from this brief, and by no means exhaustive, survey of the recrystallization literature is that unexpectedly low exponents determined by JMAK analysis of the kinetic data have been a general experimental observation, at least in plastically deformed metals. This paper attempts to account for the low exponents by exploring the effect of inhomogeneous stored energy resulting from plastic deformation. The method used is computer simulation of recrystallization where the stored energy is varied from grain to grain in the unrecrystallized structure. The remainder of this section discusses the experimental and theoretical basis for variations in stored energy in terms of dislocation and nucleus density.

An explanation for non-uniform energy storage can be found in the theory of polycrystal deformation. The Taylor model [39] postulates that all grains undergo the same macroscopic shape change. In face centered cubic metals, for example, limited slip on $\{111\}\langle 011\rangle$ slip systems results in variations in the amounts of shear or dislocation activity required to accommodate a given shape change, as a function of grain orientation. Texture prediction calculations [40] show that grain-to-grain differences in orientation lead to different accumulated total shear strains. The ratio between the magnitude of the shear sum (i.e. the sum of the individual shears on each slip system) in each grain and the magnitude of the external strain is known as the Taylor Factor. Figure 3 shows a plot of the distribution of the sum of the shears on all the slip systems for a simulated polycrystal with 200 grains at a von Mises equivalent strain of unity in plane strain compression (equivalent to a rolling reduction of 58%). This plot shows a variation of a factor of 2 between the lowest and the highest sum of the shears, reflecting the cumulative effect of the variation of Taylor Factor with orientation. Kallend and Huang [26], by detailed X-ray analysis of 50% cold rolled copper, found that the stored energy varied with orientation by a factor of four. There is also further experimental evidence for variation of stored energy in the experiments of Boas and Hargreaves [41]. They demonstrated that the microhardness of a deformed metal varied

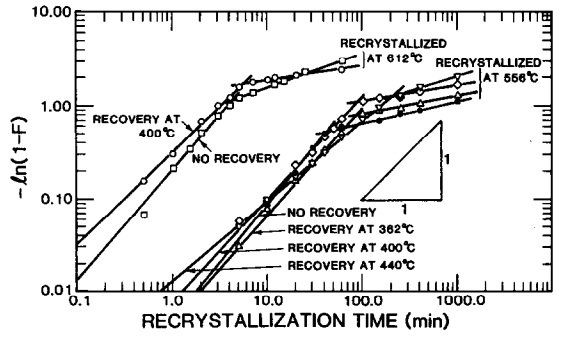

Fig. 2. JMAK plot of data for recrystallization of Fe by Rosen *et al.* [16], showing low exponents and changes in exponent during recrystallization.

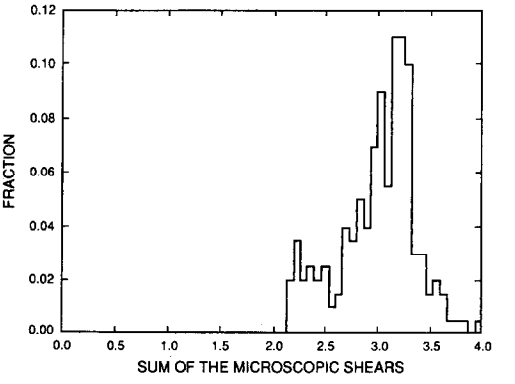

Fig. 3. Plot of the distribution of the sum-of-the-shears for a simulated polycrystal deformed to a reduction in thickness of 58%.

significantly, both within individual grains and from one grain to another. The variation in dislocation density in each grain might be expected to lead to variations in growth rate. Such variations in growth rate have been observed experimentally by Vandermeer and Gordon [42], for example. Another theoretical reason for expecting major differences in nucleation density from one grain to another is the fact that some grains in a polycrystal develop large spreads in crystallographic orientation. Bellier and Doherty investigated this in aluminum [43], and found that the transition bands between two parts of a grain that had rotated to different orientations were favorable sites for the nucleation of recrystallization. Not all the grains developed transition bands and on recrystallization after 40% compression, only some of the transition bands, in a minority of the grains, gave rise to new grains. Those that did, however, often produced clusters of nuclei [43, 44].

The next section develops two simple analytical models for recrystallization kinetics that show how non-uniform growth rates and incubation times might lower the observed JMAK exponents from the theoretical values. The following sections describe the application of a Monte Carlo model to recrystallization. The results of applying non-uniform stored energies in the model produce JMAK exponents that are very much lower than the theoretical values. These results are discussed in terms of the failure of the basic assumption of the JMAK theory of random nucleation and uniform growth.

2. ANALYTICAL MODELS

2.1. Variable nucleation and growth rate

A first step in attempting to model the recrystallization kinetics for heterogeneous nucleation and growth conditions was made by Rollett [45]. He considered a moderately deformed coarse grain polycrystal as a model material. If it is assumed that the recrystallization kinetics vary from one grain to another then a reasonable model is that of a composite material where each component or sub-volume recrystallizes at its own rate, Fig. 4. For the purposes of this development, it will be assumed that each sub-volume of the model material recrystallizes with site saturated nucleation and three dimensional growth. This would give a JMAK exponent of three if measured in each sub-volume. The kinetic equation then becomes

$$F_i = 1 - \exp(-K_i t^n). \tag{6}$$

where F_i is the fraction recrystallized for the ith sub-volume and k_i is the nucleation density and growth rate parameter for that sub-volume. For the conditions assumed here

$$k_i = (4\pi/3) I_i G_i \tag{7}$$

where I_i and G_i are the nucleation density and linear growth rate respectively for the ith sub-volume. In real materials, both the nucleation density and the growth rate might reasonably be expected to vary spatially. The kinetic equation for a composite material, where k is uniformly distributed between k_1 and k_2, is then found by taking the infinitesimal sub-volume limit in equation (6) and integrating

$$F = 1 - [\exp(-k_2 t^3) - \exp(-k_1 t^3)] t^3/(k_2 - k_1) \tag{8}$$

where the exponent, $n = 3$, has been inserted. In equation (8), k_2 corresponds to the most rapidly recrystallizing sub-volume and k_1 corresponds to the slowest. The results of employing equation (8) are shown in a JMAK plot of $\log_{10}[-\ln(1 - F)]$ vs $\log_{10}$(time), Fig. 5, where the two straight lines show the kinetics of recrystallization of the two extreme sub-volumes. A ratio of 1000 was used for k_2/k_1. The curved line in between is for the composite material and shows how the apparent exponent has the correct value, 3, at short and long times but is much lower in the transition region. A minimum value of $n \approx 0.66$ is observed. The range of F that is experimentally accessible is limited to approximately 0.1–99.9% or $\log_{10}[-\ln(1 - F)] = -3$ to 0.8. Therefore the transition from high rate recrystallization to low rate recrystallization may be spread over a sufficient range that an artifically low exponent is determined from the JMAK plot.

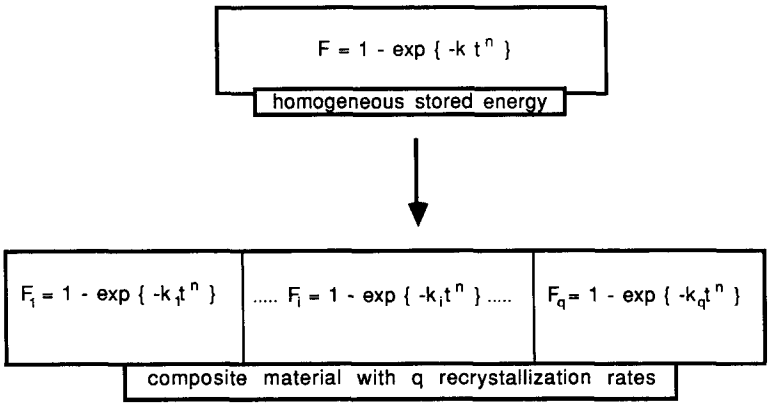

Fig. 4. Diagram of the method used to model heterogeneous nucleation and growth.

2.2. Variable incubation times

An alternative model for recrystallization kinetics in an inhomogeneous material that also produces low values of the JMAK exponent is one based on variable incubation times. In this case it is assumed that the kinetics of recrystallization are identical in each subvolume except that there is a delay, or incubation time, in the onset of nucleation in each subvolume. The form of the kinetic equation for the composite is then

$$F = 1 - \sum_i \exp - [k(t - \theta_i)^n] \qquad (9)$$

where θ_i is the incubation time of the ith subvolume and the other symbols have their previous meanings. To obtain numerical results, the same value of the exponent was chosen ($n = 3$) and 30 subvolumes were modeled whose incubation times varied linearly from 0 to a time comparable with the time required for 63% recrystallization in one subvolume, i.e.

$$\theta_{\text{maximum}} = k^{1/n}. \qquad (10)$$

The results are plotted on a JMAK plot in Fig. 6 which shows a slope that is considerably less than the value of 3 that is appropriate to each subvolume. The form of the curve is the same as for the previous model, that is, there is a transition from high to low to high slope. In contrast to the previous results, however, the range of F over which a low slope occurs is the experimentally accessible range of $F = 0.1$ to 99.9%. In the limit of infinitesimally small subvolumes and a range of incubation times much larger than the time available for measurement of F, the exponent will be one.

The major limitation of these simple models is that they take no account of the fact that recrystallized grains in a rapidly recrystallizing subvolume may grow into a neighboring subvolume that is not recrystallizing as rapidly. For this reason a Monte Carlo model was employed as described below.

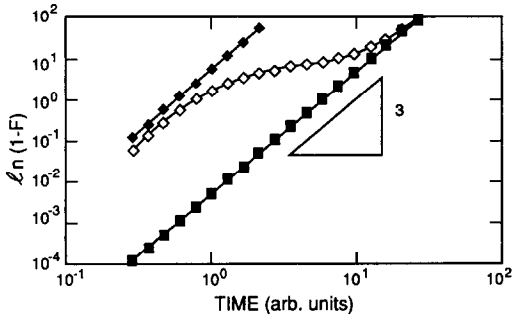

Fig. 5. JMAK plot of the kinetics of recrystallization of three model materials. Straight lines plotted with solid symbols correspond to two conditions of homogeneous nucleation and growth where $k_2/k_1 = 1000$. The curve plotted with hollow symbols corresponds to a material where there is a spatial variation of the nucleation and growth parameter, k, over the same range. The result shows a significant decrease of the apparent JMAK exponent over a certain range of volume fraction recrystallized.

3. MONTE CARLO MODEL

In order to examine heterogeneous recrystallization, the Monte Carlo model of grain growth [1] and recrystallization [2] developed by Anderson, Srolovitz, Grest and Sahni was used. This model has been shown to be highly successful in simulating the morphology, topology, kinetics and grain size distributions for grain growth [1, 46–49]. For recrystallization [2], it was shown that the model accurately simulated the kinetics of recrystallization as predicted by the JMAK equation in the limit of homogeneous stored energy. Only one change was made to the computer code to simulate the effect of heterogeneous stored energy. This was to impose a stored energy on the unrecrystallized structure that was a function of the orientation of the grain. Previous use of the model [2] had employed a single value of the stored energy imposed over the entire unrecrystallized structure.

The Monte Carlo simulation is performed on a triangular lattice of size 200 × 200 sites with periodic boundary conditions. Each ith site is assigned an orientation number, S_i. It was found that including $Q = 48$ different grain orientations was sufficient to model grain growth [50]. A grain boundary is considered to exist between site i and a neighboring site j if S_i differs from S_j. Each unlike pair of nearest neighbors is assigned an energy, J, so that the total energy of the system, E, is calculated as

$$E = J \sum_i \sum_j^{NN} (1 - \delta_{S_i S_j}) \qquad (11)$$

where the sum on i is over all 40,000 sites, the sum on j is over the nearest neighbor sites ($1 \ldots NN$) of i, and δ_{ij} is the Kronecker delta. Grain growth is simulated by permitting the orientation of a particular site to change to that of a neighboring site, provided that the total energy is reduced or left unchanged as a result of the change in orientation. The unit of time is defined in these simulations to be the Monte Carlo Step (MCS) which is the number of reorientation events, divided by the number of lattice sites (40,000).

Primary recrystallization is modeled in the same way as previously described [2, 49] in the studies of abnormal grain growth and primary recrystallization. Each distinct grain of the unrecrystallized structure, obtained from a previous grain growth simulation, is assigned a stored energy, H. The unrecrystallized grains are distinguished from the recrystallized ones by using values of S for the recrystallized grains that are larger than Q, the largest orientation number in the initial, unrecrystallized structure. Whenever a site changes orientation from an unrecrystallized value of S to a recrystallized value, the stored energy, H, at that site is liberated, i.e. the total energy is decreased by H, in addition to whatever change in grain boundary configuration there may have been. The total

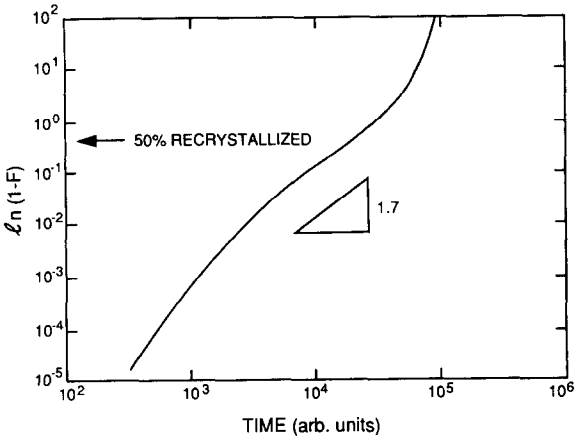

Fig. 6. JMAK plot of a model material in which the incubation time varies significantly from part of the material to another. Again, the apparent JMAK exponent is lower than the value used within each sub-volume of the material.

energy, E, of the system is then calculated as

$$E = J \sum_{i} \sum_{j}^{NN} (1 - \delta_{S_i S_j}) + Hf(S_i) \qquad (12)$$

where the function f is one for $S_i \leqslant Q$ (unrecrystallized) and zero for $S_i > Q$ (recrystallized) and the other terms of the equation are as defined in equation (11).

The essential change made for this work was to employ an H that depended on the orientation number, S_i, of the grain. Given a maximum value of stored energy, $H_{\max}$, the stored energy at an unrecrystallized site ($S_i \leqslant Q$) is chosen to vary with orientation number as

$$H_i = H_{\max} S_i / Q \qquad (13)$$

and the total energy is given by equation (12) above, except that $H = H(S_i)$. For most of the simulations described below, the stored energy was varied over a range of 0.1 ($S_i = 1$) to 5.01 ($S_i = Q = 48$). As with previous work, each calculation was repeated with five different initial structures in order to improve the statistics of the results. The physical analogue is that of examining five different regions of a material.

Nucleation is modeled by placing a nucleus, of size three lattice sites, on an arbitrary position on the lattice. Two types of nucleation conditions were modeled here. Site saturated nucleation was modeled by adding a fixed number of nuclei to the lattice at the beginning of the stimulation. Continuous nucleation was modeled by attempting to add a certain number of nuclei to the lattice at each Monte Carlo step. The essential feature of this condition is that if the nucleation attempt occurs at recrystallized sites or a site with very low stored energy, the nucleus is sub-critical and decays away. Hence the actual nucleation rate decreases with time as the fraction recrystallized increases. This corresponds to the assumptions used in deriving the JMAK equation.

Nucleation also depends on the ratio of the local stored energy to the grain boundary energy, as discussed by Srolovitz *et al.* [2, 51]. The critical homogeneous nucleus size, i.e. the smallest nucleus that can grow, is three sites for $H/J > 2$. This was the nucleus size used in this work. If H/J is less than 2, a nucleus can only survive if it is adjacent to an existing boundary. Srolovitz *et al.* [2] have shown that the growth rate of a nucleus is higher for $H/J = 5$ than for $H/J = 3$ by a factor of about 5. In a subsequent paper [51] it was shown that grains with $H/J < 2$ can initially sustain growth only along their boundaries. Furthermore [51] invasion of such grains can only occur once the nucleus straddles a vertex of the unrecrystallized grain. Therefore grains with $H/J < 2$ can only be recrystallized by nuclei forming in adjacent grains and growing to the point where they straddle a vertex. In the current simulations the stored energy was varied from grain to grain over the range 0.1–5.01. Therefore variations are anticipated in both nucleation and growth rates because the range includes the critical value of $H/J = 2$. It is suggested below that observed changes in slope of the JMAK plots are connected with these variations in nucleation and growth rates.

4. SIMULATION RESULTS

4.1. Site saturated nucleation

A plot of fraction recrystallized versus time, F vs t, for site saturated nucleation with five different numbers of initial nuclei, 100, 200, 500, 1500 and 3500 nuclei is shown in Fig. 7. The plots have a truncated sigmoidal shape that lacks the usual lead-in with small slope at short times. This lack of sigmoidal shape at early times is because of the low slopes of the JMAK plots. By differentiating equation (3) it can be seen that if $n < 1$, the slope of a plot of F vs time will decrease monotonically. If $n > 1$, however, dF/dt first increases and then decreases, giving the conventional sigmoidal shape.

The temporal evolution of the microstructure is illustrated in Fig. 8 for the case of 500 initial nuclei.

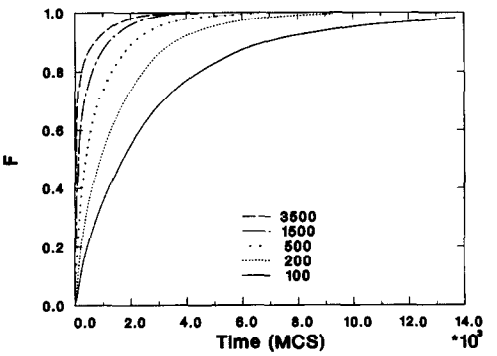

Fig. 7. Plot of fraction recrystallized, F, vs time for the Monte Carlo model undr site saturated conditions with 100 (slowest rate), 200, 500, 1500 and 3500 (highest rate) nuclei present initially.

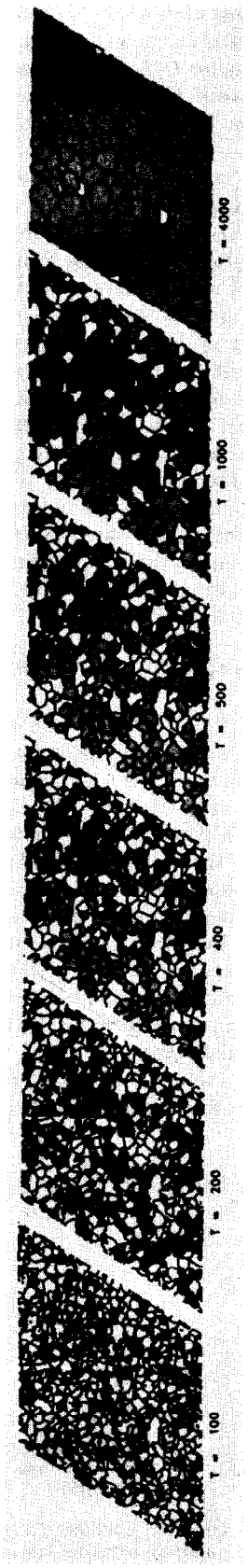

Fig. 8. Evolution of the microstructure under site saturated conditions with 500 nuclei at the beginning of recrystallization. Recrystallized grains are shaded.

The shaded grains are recrystallized grains whereas the unshaded grains are unrecrystallized. The microstructures at long times have a similar appearance to those observed experimentally. This suggests that the introduction of inhomogeneous stored energy has not affected the ability of the model to produce realistic microstructures. Elongated grain shapes do occur in the recrystallized regions but these are eventually spheroidized by grain growth in the recrystallized regions. A consequence of the variable stored energy appears to be that, although recrystallization is rapid in a few areas, small values of H in other areas result in a delay of the completion of recrystallization. This allows time for grain growth to occur to a significant extent which produces final microstructures with regularly shaped grains. This is in contrast to the results of the homogeneous stored energy case studied previously [2] where the final microstructures were found to have irregularly shaped grains. An interesting feature of the microstructures obtained under homogeneous stored energy conditions [2] was that the edges of the rapidly growing recrystallized grains contained pockets of unrecrystallized material, which Srolovitz *et al.* [2] referred to as "granulation". Although this feature can be seen at very short times, Fig. 8 ($t = 100$, 200), it rapidly disappears.

Figure 9 shows a JMAK plot of the kinetics of recrystallization under conditions of inhomogeneous stored energy for the five different numbers of initial nuclei. The slope of each line corresponds to the exponent, n, of the JMAK equation, equations (4) and (5). The expected exponent for these two-dimensional nucleation and growth conditions is 2, as was found for homogeneous stored energy [2]. The minimum slope for each line in Fig. 9, however, varies from a low of 0.4 for the largest number of initial nuclei (1500) to a high of 0.9 for the smallest number of initial nuclei (100). These exponents are very much lower than the theoretical value and are consistent with the results of the analytical model.

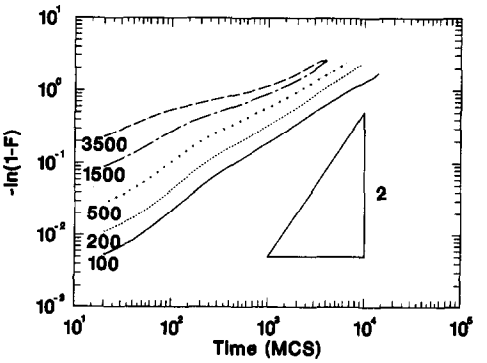

Fig. 9. JMAK plot of the results of the Monte Carlo model under site saturated conditions with 100 (lowest curve), 200, 500, 1500 and 3500 (uppermost curve) nuclei present initially. The slopes of the curves are all less than 1 in contrast to the theoretically expected value of 2 for these conditions.

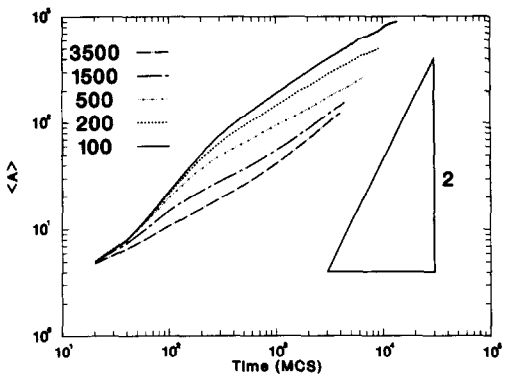

Fig. 10. Double-logarithmic plot of mean area, $\langle A \rangle$, vs time for site saturated conditions with 100 (uppermost curve), 200, 500, 1500 and 3500 (lowest curve) nuclei present initially.

described above. Figure 8 also shows that the slope is not constant during recrystallization but generally has a minimum at intermediate times. The transition from the higher slope at small values of F to the minimum slope at intermediate values of F, shifts to higher fractions recrystallized (longer times) as the nucleation density increases. This feature of the JMAK plots also occurred in the simulations of continuous nucleation described below where it is discussed further.

A logarithmic plot of the mean recrystallized grain area versus time for the five nucleation densities under site saturated conditions is shown in Fig. 10. The largest slope observed is 1.25 for the smaller nucleation densities. This is significantly less than the expected slope of 2 of un-impinged new grains growing in two dimensions which would be expected at short times. It is also apparent that the slopes of the plots are similar at long times in all five cases. This suggests an influence of grain growth on the final microstructures.

4.2. *Continuous nucleation*

The fraction recrystallized versus time for five different rates of attempted nucleation, 0.5, 2, 10, 25 and 100 nuclei added per MCS is plotted in Fig. 11. The plots have a very similar appearance to those for the site saturated case.

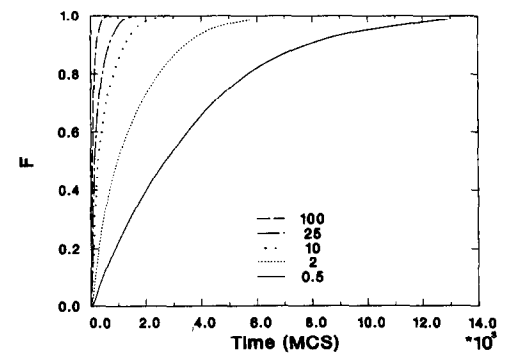

Fig. 11. Plot of fraction recrystallized, F, vs time for the Monte Carlo model under continuous nucleation conditions with nucleation rates of 0.5 (lowest rate), 2, 10, 25 and 100 (highest rate) nuclei per MCS.

Figure 12 illustrates the temporal evolution of the microstructure in a simulation with a nucleation rate of 10 per MCS. As with the site saturated case, the effect of grain growth is to promote compact grain shapes. An interesting feature of the large variations in stored energy is that there are areas where the stored energy is just sufficiently large to support the introduction of a nucleus but not large enough for the nucleus to grow appreciably. This is particularly apparent at short times where there are several unrecrystallized (unshaded) grains that have a number of very small recrystallized grains (nuclei) in their interior. The granulation that was a feature of the simulations of recrystallization [27] with large homogeneous stored energies is only observable at very short times, Fig. 12 ($t = 100$). As with the site saturated case, the end of recrystallization is prolonged by the existence of pockets of material that are very slow to recrystallize, Fig. 12 ($t = 2500$). These pockets of unrecrystallized material are areas where the stored energy is too low to support homogeneous nucleation and rapid growth. This is in contrast to the homogeneous stored energy case where continuous nucleation fills in the pockets.

JMAK plots for the five different nucleation rates are shown in Fig. 13. Once again, the slopes of the plots are very much lower than the predicted value which in this case is 3. This theoretical value, it should be noted, was accurately reproduced in the previous simulations carried out with homogeneous stored energy [2]. The slope of the curve for each nucleation rate, measured at $F = 63\%$ $[-\ln(1-F) = 1]$, varies from a low of 0.76 for the highest nucleation rate (100 per MCS) to a high of 1.16 for the smallest nucleation rate (0.5 per MCS). Although all the plots show some variation of slope, at no point do any of the plots approach the theoretical slope of 3. Again the effect of heterogeneous stored energy has been to drastically lower the apparent exponent as determined from a JMAK plot.

A logarithmic plot of the mean recrystallized grain area, $\langle A \rangle$, vs time for the five different nucleation rates is shown in Fig. 14. In contrast to the site standard case, all five plots follow a similar course with the lowest nucleation rate case reaching the largest grain size before recrystallization is complete. The slope at large times is slightly less than unity which is consistent with the early time grain growth rate previously reported for this model [1].

5. OTHER SIMULATIONS

The simulations described so far used a large enough range of stored energy that both the growth rate varied and the nucleation varied from homogeneous in high H/J regions to only heterogeneous in

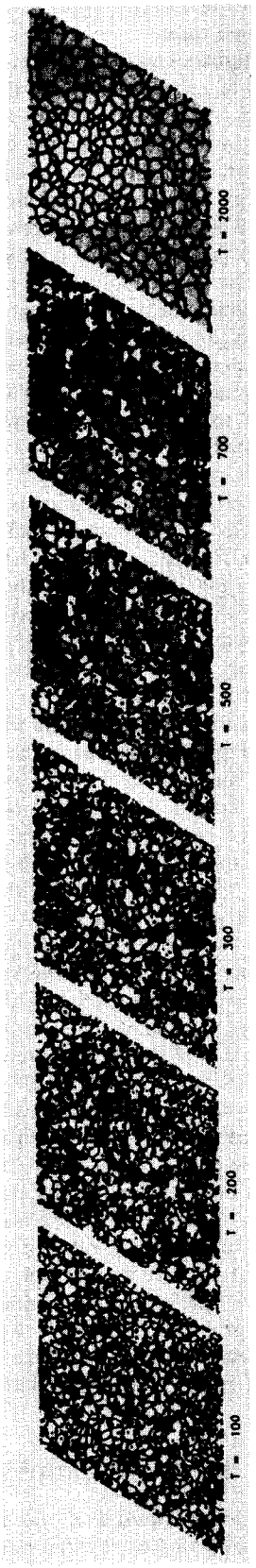

Fig. 12. Evolution of the microstructure under continuous nucleation conditions at a nucleation rate of 10 per MCS. Recrystallized grains are shaded.

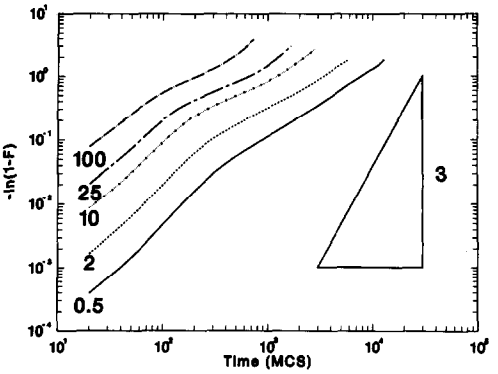

Fig. 13. JMAK plot of the results of the Monte Carlo model under continuous nucleation conditions with nucleation rates of 0.5 (lowest curve), 2, 10, 25 and 100 (uppermost curve) nuclei per MCS. The slopes of the curves are all less than 2, in contrast to the theoretically expected value of 3 for these conditions of nucleation and growth.

low H/J regions. Both the site saturated and the continuous nucleation cases produced JMAK plots with pronounced "knees" part-way through recrystallization. The effect of nucleation conditions on this transition was investigated by varying the range of stored energy at fixed nucleation rate (i.e. 25 attempts per MCS). In the one case, H/J was varied from 0.1 to 1.99 such that only heterogeneous nucleation was possible, which resulted in a minimum slope of 1.1. In another case, H/J was varied from 2.01 to 5.01 so that all unrecrystallized grains would support homogeneous nucleation, which resulted in a minimum slope of 2. Figure 15 shows a JMAK plot of the results of these two simulations, together with the results of the simulation for 25 attempts per MCS shown in Fig. 13, which resulted in a minimum slope of 0.71. In addition, Fig. 15 shows a curve for the results of a further simulation with the same nucleation conditions but a smaller range of stored energy, $H/J = 0.5$ to 5.01, which resulted in a minimum slope of 0.74. It is clear that when the nucleation conditions are such that nucleation is either entirely homogeneous, $2 \leqslant H/J \leqslant 5$, or entirely heterogeneous,

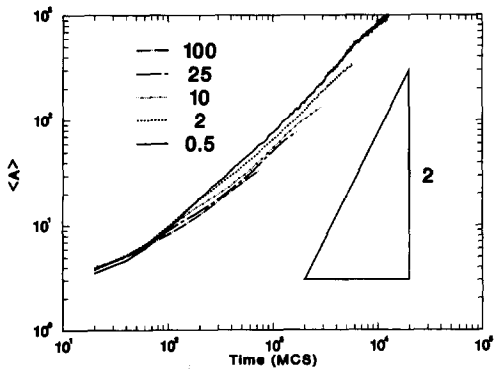

Fig. 14. Double-logarithmic plot of the mean grain area vs time for conditions of continuous nucleation with nucleation rates of 0.5 (uppermost curve), 2, 10, 25 and 100 (lowest curve) nuclei per MCS.

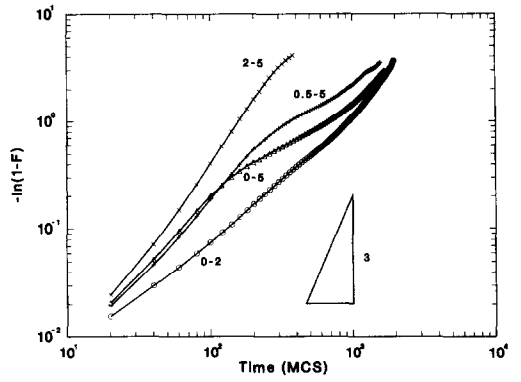

Fig. 15. JMAK plot of recrystallization under continuous nucleation at a rate of 25 per MCS with stored energy ranges of $0 \leqslant H/J \leqslant 1.99$ (lowest curve), $0 \leqslant H/J \leqslant 5$, $0.5 \leqslant H/J \leqslant 5$ and $2 \leqslant H/J \leqslant 5$ (uppermost curve).

$0 \leqslant H/J \leqslant 2$, no "knee" or transition in slope is observed. The next-to-lowest curve where nucleation conditions are mixed, $0 \leqslant H/J \leqslant 5$, shows a pronounced knee. This knee is tentatively ascribed to a transition from recrystallization dominated by homogeneous nucleation and rapid growth at short times, to recrystallization dominated by heterogeneous nucleation and slower growth at long times. The curve for the smaller range of stored energy, $0.5 \leqslant H/J \leqslant 5$, shows that the knee is not sensitive to the exact range of H/J used. Such transitions have been frequently observed experimentally, as can be seen in the JMAK plots of Rosen *et al.* [16], Fig. 2, or Vandermeer and Gordon [36].

Simulations were also performed under conditions of homogeneous stored energy but limiting nucleation to a small minority of grains. This results in clustering of the nuclei, early impingement of the recrystallizing grains and a transient decrease in slope of the JMAK plot.

6. THE JMAK EQUATION

The JMAK equation depends fundamentally on the differential relationship between actual volume fraction recrystallized and the extended volume, equation (1). If this equation does not hold then the JMAK theory is not an adequate description of the kinetics of recrystallization. One possible variant of equation (1) has been worked out in detail by Gokhale *et al.* [52] where a particular clustering of nuclei was assumed. Their model does not appear to be generally applicable, however.

In order to test equation (1) for the site saturated case (Section 4.1) two further sets of simulations were performed in which only one, new (recrystallized) grain was introduced. These single grain simulations were performed in order to estimate the "extended volume fraction" in multi-grain simulations. As in all the simulations, five different initial microstructures derived from grain growth simulations were used to obtain improved statistics. The first set used a homogeneous stored energy, $H/J = 3$ and the second set used the same range of stored energy as employed in the site saturated simulations of Section 4.1, i.e. $0.1 \leqslant H/J \leqslant 5$. The results of these simulations were used to determine the growth rate of a single recrystallized grain. Since, in this case, no impingement with other recrystallized grains occur until the single grain reaches the edges of the lattice and impinges on itself, the volume fraction, F_1, at any time is equal to the extended volume fraction [F_e in equation (1)]. Therefore, from this simulation we calculate an extended volume fraction, F_e, from which dF_e/dt was obtained by differentiation. If the single grain volume fraction is F_1 and the number of grains in the multi-grain simulation is m

$$F_e = mF_1. \tag{14}$$

The results of a previous simulation of recrystallization [2] with homogeneous stored energy, $H/J = 3$ and 500 nuclei (site saturated) were used to calculate dF/dt. The test of equation (1) was made by using the ratio of dF/dt to the extended volume growth rate, dF_e/dt, obtained from the single grain simulations described above. Figure 16 shows a logarithmic plot of $[(dF/dt) \div (dF_e/dt)]$ vs $(1 - F)$. The straight line on this plot is the relationship of equation (1). The result of this test is clearly that the main assumption of the JMAK theory is valid for the Monte Carlo model of recrystallization under conditions of homogeneous stored energy. This is, of course, as expected in view of the good agreement between theory and simulation for the JMAK exponents found by Srolovitz *et al.* [2].

When the same comparison of $[(dF/dt) \div (dF_e/dt)]$ *vs* $(1 - F)$ is made for the case of heterogeneous stored energy conditions and 3500 nuclei, Fig. 17, the results are dramatically different. The line of equation (1) is close to the simulation results at $1 - F \sim 1$

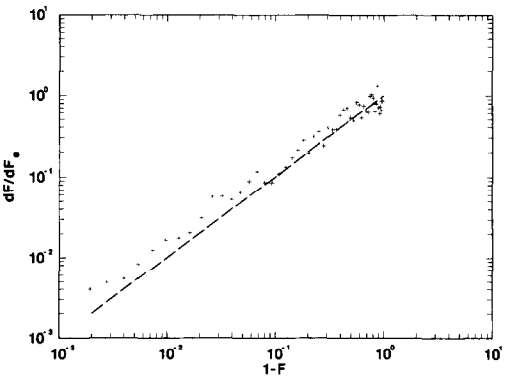

Fig. 16. Double-logarithmic plot of the ratio of rate of increase of actual fraction recrystallized to extended fraction, versus 1-F for conditions of site saturation with 200 nuclei and homogeneous stored energy, $H/J = 3$. Equation 1 is plotted as a dashed line and the coincidence of the results with the theoretical prediction indicates that the basic assumption of the JMAK theory is correct.

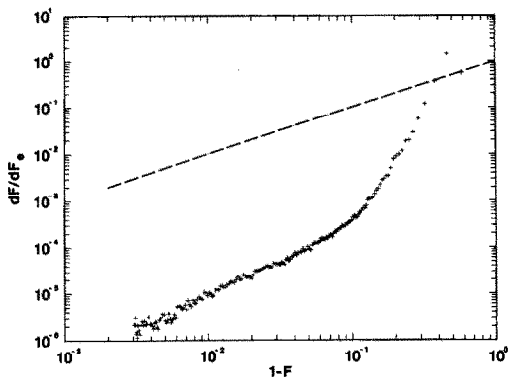

Fig. 17. Double-logarithmic plot of the ratio of rate of increase of actual fraction recrystallized to extended fraction, versus 1-F for conditions of site saturation with 3500 nuclei and heterogeneous stored energy, $H/J = 0$–5. The slope is much greater than one at all times and indicates a departure from the basic assumption of the JMAK theory, Eq. 1 (dashed line).

within the statistical scatter. However, the simulation data rapidly fall below the values predicted by equation (1), by a factor of 10 at $1 - F = 0.25$ and by two orders of magnitude at $1 - F = 0.15$. That is, equation (1) gravely underestimates the impingement correction in the case of heterogeneous stored energy. Similar discrepancies were observed for different nucleation densities. This result shows that the reason for the low JMAK exponents observed in these simulations is the failure of the key assumption of the JMAK theory, that is, spatially random nucleation and uniform growth. This suggests that the JMAK analysis is not appropriate for recrystallization of plastically deformed materials which almost inevitably have non-uniform stored energies.

7. CONCLUSIONS

The conclusions from this work can be stated as follows:

The significance of inhomogeneous stored energy (from deformation) has been demonstrated for the process of primary recrystallization. The inhomogeneity of stored energy arises from the anisotropy of dislocation-controlled slip which gives rise both to grain-to-grain differences in predicted total shear and to differences in measured stored energy. Such inhomogeneity also appears to give rise to nucleation densities that vary from one grain to another.

Inhomogeneous stored energy can lead to Avrami exponents (i.e. the slope in the JMAK plots) that are much lower than those theoretically predicted for the given nucleation and growth conditions. The low exponents obtained from the simulations are similar to the results observed in many experiments.

The reason for the low JMAK exponents in the inhomogeneous stored energy case appears to be the failure of the differential equation, equation (1), used to derive all the various forms of the JMAK equation, equation (4). In the limit of homogeneous stored energy, however, a test of equation (1) showed that it is valid over a large range of fraction recrystallized.

The exponents observed in the simulation decrease with decreasing grain size in the recrystallized state. This trend is in the same direction as observed experimentally where high exponents were obtained for small pre-strains, leading to a recrystallized grain size that was coarse compared to the prior grain size. When large prestrains were used, however, such that the recrystallized grain size was comparable to the initial grain size, low exponents were typically obtained experimentally.

Transitions or "knees" in the JMAK plots are a characteristic feature of primary recrystallization with inhomogeneous stored energy and occur at fractions recrystallized that increase with the nucleation density. This feature is also commonly observed experimentally.

Grain growth is significant when primary recrystallization is slowed by the presence of "hard to recrystallize" (i.e. low stored energy) regions of the microstructure. Grain growth coarsens the recrystallized grain structure while the transformation is going to completion in the unrecrystallized regions.

Acknowledgements—The authors gratefully acknowledge fruitful discussions with J. D. Embury, W. G. Fricke, L. Lalli, J. Liu, S. Pancha, V. M. Sample, M. A. Zaidi and U. F. Kocks. A.D.R. and D.J.S. were supported by the U.S. Dept. of Energy through the Los Alamos National Laboratory.

REFERENCES

1. M. P. Anderson, D. J. Srolovitz, G. S. Grest and P. S. Sahni, *Acta metall.* **32,** 783 (1984).
2. D. J. Srolovitz, G. S. Grest and M. P. Anderson, *Acta metall.* **34,** 783 (1986).
3. J. W. Christian, *The Theory of Phase Transformations in Metals and Alloys*, Part I. Pergamon Press, New York (1975).
4. M. Avrami, *J. chem. Phys.* **7,** 1103 (1939).
5. M. Avrami, *J. chem. Phys.* **8,** 212 (1940).
6. M. Avrami, *J. chem. Phys.* **9,** 177 (1941).
7. W. A. Johnson and R. F. Mehl, *Trans. Am. Inst. Min. Engrs* **135,** 416 (1939).
8. A. E. Kolmogorov, *Akad. nauk SSSR, Izv., Ser. Mat.* **1,** 355 (1937).
9. J. W. Cahn, *Acta metall.* **4,** 449 (1956).
10. W. G. Fricke and H. B. McShane, in *Textures in Non-ferrous Metals and Alloys* (edited by H. D. Marchant and J. G. Morris), pp. 17–51. TMS-AIME, Warrendale, Pa (1985).
11. W. A. Anderson and R. F. Mehl, *Trans. Am. Inst. Min. Engrs* **161,** 140 (1945).
12. R. D. Doherty, *Recrystallization of Metallic Materials* (edited by F. Haessner), p. 23. Riederer, Stuttgart (1978).
13. P. Gordon, *J. Metals* **201,** 1043 (1955).
14. A. Galibois and A. Dube, *Can. Metall. Q.* **3,** 321 (1964).
15. J. T. Michalak and W. R. Hibbard, *Trans. Am. Soc. Metals* **53,** 331 (1961).

16. A. Rosen, M. S. Burton and G. V. Smith, *Trans Am. Inst. Min. Engrs* **230,** 205 (1964).
17. E. C. W. Perryman, *Trans. A.I.M.E. J. Metals* **203,** 369 (1955).
18. P. Faivre, D. Phil. thesis, Sussex Univ., England (1973).
19. D. Juul Jensen, N. Hansen and F. J. Humphreys, *Acta metall.* **33,** 2155 (1985).
20. P. A. Comte and W. Form, *Z. Metallk.* **67,** 158 (1976).
21. R. A. Petkovic, M. J. Luton and J. J. Jonas, *Acta metall.* **27,** 1633 (1979).
22. M. J. Luton, R. A. Petkovic and J. J. Jonas, *Acta metall.* **28,** 729 (1980).
23. N. Hansen, T. Leffers and J. K. Kems, *Acta metall.* **29,** 1523 (1981).
24. W. C. Setzer and J. G. Morris, *Trans. Am. Soc. Metals* **57,** 589 (1964).
25. P. Laurent and M. Batisse, *Rev. Metall.* **46,** 485 (1952); *ibid.*, p. 593.
26. J. S. Kallend and Y. C. Huang, *Metal Sci.* **18,** 381 (1984).
27. C. Carmichael, A. S. Malin and M. Hatherly, *ICSMA-6,* Sydney, Australia, Vol. 1, p. 381 (1981).
28. Y. Inokuti and R. D. Doherty, *Acta metall.* **26,** 61 (1978).
29. F. Adcock, *J. Inst. Metals* **27,** 73 (1922).
30. J. D. Embury and E. Koken, unpublished research.
31. E. Nes and J. K. Solberg, *Mater. Sci. Tech.* **2,** 19 (1986).
32. D. Akhtar, *Scripta metall.* **20,** 983 (1986).
33. I. S. Servi and D. Turnbull, *Acta metall.* **14,** 161 (1966).
34. M. E. Fine, *Introduction to Phase Transformations in Condensed Systems.* MacMillan, New York (1964).
35. C. Wert and C. Zener, *J. appl. Phys.* **21,** 5 (1950).
36. R. A. Vandermeer and P. Gordon, *Symposium on the Recovery and Recrystallization of Metals,* p. 211. T.M.S.-A.I.M.E., New York (1962).
37. P. Shewmon, *Transformation in Metals.* McGraw-Hill, New York (1969).
38. E. C. W. Perryman, *Trans. A.I.M.E. J. Metals* **203,** 1053 (1955).
39. G. I. Taylor, *J. Inst. Metals* **62,** 307 (1938).
40. G. R. Canova, U. F. Kocks and J. J. Jonas, *Acta metall.* **32,** 211 (1984).
41. W. Boas and M. E. Hargreaves, *Proc. R. Soc.* **A193,** 89 (1948).
42. R. A. Vandermeer and P. Gordon, *Trans. Am. Inst. Min. Engrs* **215,** 577 (1959).
43. S. Bellier and R. D. Doherty, *Acta metall.* **25,** 521 (1977).
44. S. Bellier, Ph.D. thesis, Sussex Univ., England (1971).
45. A. D. Rollett, M. S. thesis, Drexel Univ. (1986).
46. D. J. Srolovitz, M. P. Anderson, P. S. Sahni and G. S. Grest, *Acta metall.* **32,** 793 (1984).
47. D. J. Srolovitz, M. P. Anderson, G. S. Grest and P. S. Sahni, *Acta metall.* **32,** 1429 (1984).
48. G. S. Grest, D. J. Srolovitz and M. P. Anderson, *Acta metall.* **33,** 509 (1985).
49. D. J. Srolovitz, G. S. Grest and M. P. Anderson, *Acta metall.* **33,** 2233 (1985).
50. P. S. Sahni, D. J. Srolovitz, G. S. Grest, M. P. Anderson and S. A. Safran, *Phys. Rev. B* **28,** 2705 (1983).
51. D. J. Srolovitz, G. S. Grest, M. P. Anderson and A. D. Rollett, *Acta metall.* **36,** 2115 (1988).
52. A. M. Gokhale, C. V. Iswaran and R. T. deHoff, *Metall. Trans.* **11A,** 1377 (1980).