A general approach to grain growth driven by energy density differences

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Abstract

A general approach to grain growth driven by energy density differences among the grains, associated with curvature and/or extraneous driving forces (e.g. external fields) is developed. A mean field approximation leads to the definition of a threshold energy density, $E^*$, which depends on moments of the current distributions of grain diameters, $a$, and grain energy densities, $E$, such that the rate of change, $\frac{da}{dt}$, of the diameter of a grain is proportional to $(E^*-E)$. When curvature effects are negligible, the kinetic equations can be solved analytically to obtain the average grain diameter and the diameter distribution as a function of time. A scaling regime is reached for (and only for) power law distributions of $E$, with a power law kinetics $\langle a \rangle \propto t^\mu$. The combined effects of curvature and extraneous driving forces were studied numerically. The rate of growth and the width of the grain diameter distribution change when compared to pure curvature growth, the sign of the change depending on the initial energy density and diameter distributions. © 2002 Acta Materialia Inc. Published by Elsevier Science Ltd. All rights reserved.

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1. Introduction

1.1. Phenomenology of grain growth

In the absence of other driving forces, grain growth in a polycrystal is driven by the curvature of the grain boundaries. A simple kinetic equation, first proposed by Hillert [1], is often used for the rate of change of the grain diameter, $a$, in curvature driven growth

$$\frac{da}{dt} = k' \left( \frac{1}{a^*} - \frac{1}{a} \right); \quad k' = \varphi M' \gamma. \quad (1)$$

The kinetic constant $k'$ is proportional to the mobility $M'$ of the boundaries, to their specific free energy $\gamma$ and to a geometrical factor $\varphi$, all assumed to be the same for all boundaries. The quantity $a^*$ is a threshold diameter, such that, at any time $t$, grains with $a > a^*$ grow and grains with $a < a^*$ shrink and eventually disappear. Since the total size (volume or area, respectively, for three dimen-
Grain growth governed by eq. (1) may lead to a scaling regime [2,3], in the sense that the distribution of $a/\langle a \rangle$ becomes time invariant (steady state). In this scaling regime, the average diameter $\langle a \rangle$ increases with $t^{1/2}$ (parabolic kinetics) both in 2D and 3D polycrystals [2]. In general, experimental observations reveal power law exponents smaller than 1/2 [4], which are usually attributed to various effects, such as boundary tension inhomogeneity or a drag effect caused by impurities, which are not taken into account in the simple eq. (1).

One possible distribution of grain diameters in the scaling regime was found by Hillert [1] and will be referred to as the Hillert distribution. It has been shown that other steady state distributions exist [2,3] forming a one parameter family.

In addition to the driving force provided by the curvature effect, there may be additional or extraneous driving forces for grain growth whenever there is a difference in the energy densities among the grains, as for example when an external electric or magnetic field is present. In such cases, the energy density, $E$, can be written in the form

$$E = -PF$$

where $F$ is the external field intensity (assumed uniform) and $P$ is an electrical polarization or magnetization, either permanent or induced by $F$. For permanent moments, $P$, with a definite crystallographic orientation in the grains,

$$E \propto -\cos \theta$$

where $\theta$ is the angle between $F$ and $P$; the distribution of $\theta$ is determined by the orientation of the grains. If $P$ is induced by $E$, then, in general,

$$P = \psi(\alpha)F,$$

where $\psi(\alpha)$ is a grain orientation dependent susceptibility, and

$$E \propto \psi(\alpha)F^2.$$  \hspace{1cm} (4)

There are other situations where differences in the energy density of the grains are caused by or associated with elastic strains due to an applied stress or to residual stresses; or to differences in the surface energy (e.g., in thin films). Many examples of the effects of these extraneous driving forces on grain growth and grain boundary mobility can be found in the literature, which we briefly review in the following section.

1.2. Effects of extraneous driving forces in grain growth

Among the first experiments on the effect of an extraneous driving force in grain growth, Mullins et al. [5,6] have investigated the effect of a magnetic field (7–8 T) on the grain boundary velocity and consequent effect on grain growth in bismuth. They found that the presence of a magnetic field induces growth in grains with specific orientations. Watanabe et al. [7], and Martikainen and Lindros [8] reported that a magnetic field applied to a polycrystal during annealing affects the kinetics of grain growth and texture. Ohtachi [9] found that after annealing a Fe-50% Co film under a 1.5 T field, the grain size distribution became narrower. Ono et al. [10] carried a simulation of grain growth in which the effects of surface energy and magnetic anisotropy were taken into account. When both effects were considered, a single-stage growth was observed, whereas abnormal grain growth occurred when only the magnetic field was considered. More recently, Molodov et al. [11] showed that the presence of a magnetic field provided the driving force to move a planar grain boundary in a bismuth bicrystal. From the measured grain boundary velocity they calculated the grain boundary mobility.

Another effect was found in two studies on high-purity Cu by Conrad et al. [12,13]. They showed that high density electric current pulses retarded the grain growth rate, following the completion of recrystallization. It was suggested that the effect of electropulsing was to alter the concentration of vacancies, which then enhanced dislocation climb.
and reduced the residual dislocation density. As a result, the driving force for grain growth was reduced. Another example of an extraneous driving force for grain growth was proposed by Srolovitz et al. [14]. They suggested that differences in strain energy between grains in a polycrystalline material might also cause abnormal grain growth. The driving force is the reduction in strain energy, lead by the elimination of grains with higher residual strain. Srolovitz et al. [14] assumed that the strain energy is proportional to the dislocation density and thus there is a critical size above which the strain energy dominates over the grain boundary energy. Briant et al. [15], following the ideas of Srolovitz et al. [14], found that as deformation increases, the critical size for abnormal grain growth decreases.

Recently, Nabarro [16] considered the effect of a uniform applied stress on the process of grain growth. Induced by the presence of an applied stress, a grain A will grow at the expense of another grain B, while grain B changes orientation to that of grain A. The growth or shrinkage of the grains is determined by the sign of the strain. Volkert and Lingk [17] reported an enhancement in grain growth in Al films annealed under an applied compressive stress. Since it was shown that grain boundary mobility in Al decreases with compressive pressure [18], Volkert and Lingk [17] suggested that the acceleration of grain growth was due to an enhancement in surface planarity of the Al films. In this fashion, films with initially smooth surfaces will exhibit faster grain growth kinetics even in the absence of applied compression. Winning et al. [19] investigated the motion of planar low- and high-angle grain boundaries under an applied shear stress. Grain boundary velocities were found to depend linearly on the external stress. From measurements of the activation enthalpies of migration, they concluded that the stress driven motion of planar grain boundaries can be associated with the climb assisted motion of the dislocations which compose the boundary.

These investigations show that an extraneous driving force can play an important role in grain growth. In actual systems, the driving force due to the reduction in grain boundary energy will compete with the extraneous driving force. Thus, it is important to develop a theoretical framework to characterize the regime where these extraneous fields are seen to play a role in grain growth, in addition to, or even in substitution of, curvature. For this purpose, it seems appropriate to take the general approach of considering the material as an assembly of grains with different energy densities. We will show that an energy density associated with the curvature of grain boundaries can be attributed to each grain. The total energy density of each grain is simply the sum of the corresponding terms associated with the boundary energy and the extraneous driving forces. The purpose of this paper is to investigate the effect of these extraneous driving forces on grain growth, in addition to and/or in place of that due to curvature. We will derive a general growth equation for the rate of change of the diameter, \( a \), of a grain as a function of its energy density. We will be particularly interested in finding how the width of the diameter distribution and the global kinetics are affected by external driving forces. This will be achieved by numerical integration of the growth equation. When the curvature effect is neglected, the resulting equations can be solved analytically.

### 2. The kinetic equation

#### 2.1. Grain growth driven by differences in energy density

Consider an assembly of \( N \) grains (large \( N \)), each with size \( S_i \) (volume in 3D or area in 2D polycrystals). The total size, \( \sum_i S_i \), is time invariant. The boundary between grains \( i \) and \( j \) has extension \( l_{ij} \) (area in 3D or length in 2D). We assume that an external driving force generates in each grain a (uniform) energy density (energy per unit size) \( E_i \). The driving force is associated, for example, with a magnetic, electric or stress–strain field. The effect of curvature will not be explicitly considered at this stage.

The boundary between adjacent grains \( i \) and \( j \) moves with a velocity \( v_{ij} \), normal to the interface, given by

\[
v_{ij} = -M(E_i - E_j),
\]
where $M$ is the (constant and uniform) interface mobility. The mobilities $M$ and $M'$ (in curvature driven growth, eq. (1)) need not be equal. The boundary moves in the direction of the grain with largest energy density. For $v_{ij} > 0$, $(E_i < E_j)$, the boundary moves in the direction of grain $j$. Thus, we can write for the rate of change of the size, $S_i$, of grain $i$

$$\frac{dS_i}{dt} = \sum_j l_{ij}v_{ij},$$

where the sum includes all grains adjacent to grain $i$. Combining eqs. (5) and (6) yields

$$\frac{dS_i}{dt} = \sum_j l_{ij}v_{ij} = -M\sum_j (E_i-E_j)l_{ij},$$

which can be written as

$$\frac{dS_i}{dt} = -M(\sum_j l_{ij}(E_i-E^*_i),$$

where we introduced

$$E^*_i = \frac{\sum_j l_{ij}E_j}{\sum_j l_{ij}}.$$  

This quantity can be regarded as an average energy density of the grains adjacent to grain $i$. In a mean field approximation these quantities $E^*_i$ will be taken as identical for all grains: $E^*_i = E^*$. If we further assume that

$$\sum_j l_{ij} = \phi S_i^{n-1},$$

where $n$ is the dimensionality of the polycrystal and $\phi$ is a shape factor, the same for all grains, we can rewrite eq. (8) in the form

$$\frac{dS_i}{dt} = -k''S_i^{n-1}(E_i-E^*)$$

where $k'' = \phi M$ is a constant.

It is now convenient to introduce a grain diameter $a_i$ (which will also be referred to as grain size) defined as

$$a_i = S_i^{1/n}. $$

Eq. (11) becomes

$$\frac{da_i}{dt} = -k(E_i-E^*); \quad k = \frac{\phi M}{n}$$

and eq. (9) simplifies to

$$E^* = \frac{\sum d_i^{n-1}E_i}{\sum d_i^{n-1}} = <a^{n-1}E> <a^{n-1}>.$$ 

It is readily seen that eq. (13) with $E^*$ defined by eq. (14) leads to conservation of the total size

$$\frac{dS_{tot}}{dt} = \sum_i \frac{d a_i^i}{dt} = 0,$$

which shows the consistency of the mean field approach that was introduced. Note that the number of grains decreases but the eliminated grains have zero size.

The quantity $E^*$ can be regarded as a threshold energy, which is the average energy density weighed by the grain diameter. Thus, grains with $E = E^*$ do not change their size, grains with $E > E^*$ shrink (and eventually disappear) and those with $E < E^*$ grow. Note that $E^* = E^*(t)$ even when the $E_i$ are time independent, as will be assumed throughout this paper. Omitting the subscript $i$ in eq. (13) we write

$$\frac{da}{dt} = -k(E-E^*).$$

Eq. (1) is formally identical to eq. (16) if we define an energy density $E^* \frac{1}{a}$ (e.g., $E = \frac{\phi \gamma}{a}$) associated with grain boundary curvature. This is plausible, since the boundary energy of a grain of diameter $a$ is proportional to $\gamma a^2$, while its volume is proportional to $a^3$. If we apply eq. (14) to this case we obtain for the threshold energy

$$a^* = <a^{n-1}> <a^{n-2}>.$$ 

which coincides with the result derived in [2]. For $n = 2$ the threshold diameter $a^*$ is the average diameter $<a>$, as obtained by Hillert [1]. Despite this similarity, there is, however, a fundamental difference between the grain growth eqs.
(1) and (16). While in eq. (16) the energy density, \( E \), of a grain, associated with an external field, is a constant, in eq. (1) the energy density \( E \frac{1}{a} \) is a time dependent quantity. Nevertheless, by using the concept of energy density, we can integrate in one formalism either curvature or an external driving force. We also note that eq. (16) is formally similar to von Neumann’s equation [20]

\[
\frac{dA_n}{dt} = c(n-6), \tag{18}
\]

which states that the rate of change of the area \( A_n \) of a bubble with \( n \) sides in a 2D froth (\( n > 6 \)) is proportional to \((n-6)\). Von Neumann’s equation also applies to 2D curvature driven grain growth when there is equilibrium at triple junctions [21].

We now discuss in more detail grain growth when both effects (curvature and energy density differences) are present.

2.2. Grain growth driven by curvature and an extraneous driving force

The growth equation that takes into account curvature and (other) energy density differences can be written in the form (see eqs. (1) and (16))

\[
\frac{da}{dt} = -k'\left(1 - \frac{1}{a^2}\right) - k(E-E^*) \tag{19}
\]

assuming additivity of the driving forces [22]. The relative importance of curvature and energy differences in grain growth can be measured by the ratio

\[
R = k'/(k(<a> < E>)) \tag{20}
\]

which, in general, is time dependent. When \( R \) increases with time, curvature effects will become increasingly important and vice versa.

Eq. (19) can in principle be integrated so as to obtain the compound distributions \( h(a,E,t) \) and \( h(a,<a>,<E>,t) \) for the surviving grains at time \( t \), given the initial distributions of grain diameters and energy densities. When scaling is reached, \( h \) becomes time independent.

In the general case, analytical integration of eq. (19) seems difficult, so we have resorted to numerical simulations, for various initial distributions of diameters and energies, later presented in Section 4. It is convenient to address first the simpler problem of integration of eq. (19) in the absence of the curvature term (eq. (16)). In this case, it is possible to solve the equation analytically, as shown in the following section.

3. Absence of curvature effect

This section deals with the particular case where the curvature effect can be neglected (\( R = 0 \)). In this “pure” energy density case, the growth equation reduces to eq. (16). We will show how this equation can be handled analytically, to obtain the kinetics and other characteristics of grain growth driven by (time independent) energy density differences. In Section 3.1.1 the case where grains that are initially of the same diameter and have an arbitrary energy density distribution is treated. In Section 3.1.2 we apply the results obtained in Section 3.1.1 to power law energy distributions, which lead to a scaling regime of growth. In Section 3.2 we show that the equations obtained apply to any initial distribution of grain diameters. Finally, in Section 3.3 we show that the power law energy distributions are unique in leading to a scaling regime under the above growth law (eq. (16)).

The unit of length will be chosen as the initial average grain diameter

\[
< a > (t = 0) = 1. \tag{21}
\]

We consider a large number \((N \to \infty)\) of grains with a continuous energy density distribution defined by an initial probability density function \(f(E,0) = f(E,t = 0)\), with \( E \) in the interval [0,1]. This is equivalent to take for energy zero the lowest energy, \( E_m \), of the grains, while the energy unit is taken as the one of the (initial) highest energy grain, \( E_M \)

\[
E_m(t = 0) = 0; E_M(t = 0) = 1. \tag{22}
\]

Note that \( E_m = 0 \) at all times, but \( E_M \) is time dependent.

The normalization condition is
We introduce a reduced time, \( t \), related to real time, \( t' \), by
\[
t = kt',
\]
and write eq. (16) as
\[
\frac{da}{dt} = E^* - E.
\]

3.1. Uniform initial grain sizes

3.1.1. Arbitrary energy distributions
We first treat the case where all grains have the same initial diameter \( a = 1 \). We will also use the notation \( a_E \) for the diameter of a grain with energy \( E \). The rate of change of \( a_E \) is related to that of grain \( a_0 \) with the lowest energy \( E = 0 \), by
\[
\frac{da_E}{dt} - \frac{da_0}{dt} = -E,
\]
which integrates to
\[
a_E - a_0 = -Et,
\]
since we are assuming that all grains have the same diameter at \( t = 0 \).

At time \( t \), grains with energy above a certain \( E_M(t) \) have disappeared. \( E_M \) is the highest energy of the surviving grains at \( t \). The grains with energy \( E_M(t) \) have, of course, diameters close to zero. The energy \( E_M \) is then determined by setting \( a_{E_M(t)} = 0 \) in eq. (27) leading to
\[
E_M = a_0(t); \ t > t_1.
\]
This and the following equations apply for \( t > t_1 \), where \( t_1 \) is the (reduced) time at which the grain with highest energy, \( E = 1 \), in the initial distribution, disappears. Combining eqs. (27) and (28) we obtain
\[
a_E(t) = (E_M - E)t; \ t > t_1.
\]
When the maximum energy in the polycrystal is \( E_M(t) \), the probability density function \( f(E,t) \) of the surviving grains is
\[
f(E,t) = F^{-1} f(E,0); \ E \leq E_M(t),
\]
since there is no change in the energy density of each grain. The quantity \( F = F(t) \) is both a normalization factor
\[
F = \int_0^{E_M} f(E,0) dE,
\]
and also the fraction of surviving grains (in number \( N(t) \) at time \( t \), relative to the initial number \( N_0 \))
\[
F = \frac{N(t)}{N_0}.
\]
The total size (the total \( a^n \), where \( n \) is the dimensionality of the polycrystal) is conserved and equal to the initial total size \( S = N_0 < a^n > (t = 0) \). We then have
\[
N_0 = N_0 F \int_0^{E_M} f(E,t) a^2 dE.
\]
Combining with eqs. (29) and (30) yields, after simplification \( t^* \)
\[
\int_0^{E_M} f(E,0)(E_M - E)^n dE = 1; \ t > t_1
\]
which determines \( E_M(t) \). The original grain of highest energy density \( E = E_M(t = 0) = 1 \) is eliminated at \( t_1 \) given by eq. (34) for \( E_M = 1 \).

Combining eqs. (25) and (29) we obtain an equation for \( E^*(t) \)
\[
E^* = \frac{d}{dt} (E_M(t))
\]
where \( E_M(t) \) is defined by eq. (34). The average energy density \( <E> \) at time \( t \) is given by
\[
< E > = F^{-1} \int_0^{E_M} f(E,0) E \ dE.
\]
The average grain diameter can be calculated from
\[
< a > = \int_0^{E_M} a_E f(E,t) dE
\]
because of the one-to-one correlation between diameter and energy density expressed by eq. (29). Using eqs. (29) and (30) this gives

$$<a> = \left[ F^{-1} \int_{0}^{E_M} f(E,0)(E_M - E)dE \right] t, \quad (38)$$

which can also be written as

$$<a> = (E_M - <E>) t, \quad (39)$$

where we used eq. (36).

The probability density function \(g(a,t)\) of the grain diameters at time \(t\) can be obtained by noting that the grains in the energy interval \(E, E + dE\) (in number \(N_0 f(E,t)dE\)) are exactly in the grain diameter interval between \(a_E\) and \(a_E + da_E\), with \(d\alpha E = t dE\) (eq. (29) at fixed time and therefore fixed \(E_M\)). Thus

$$g(a,t) = \frac{f(E,t)}{t} = \frac{F^{-1} f(E,0)}{t}, \quad (40)$$

with \(E\) related to \(a\) = \(a_E\) and \(t\) by eqs. (29) and (34). The distribution of reduced grain diameters, \(g_r(a) = \frac{a}{<a>} t\), can be obtained from \(g(a,t)\)

$$g_r(a) = \frac{a}{<a>} t = <a> g(a,t) = \frac{<a>}{t} F^{-1} f(E,0). \quad (41)$$

It is of interest to introduce the variance, \(s^2\), of the diameter distribution, which measures the width of the distribution

$$s^2 = \frac{<(a - <a>)^2 >}{<a>^2} \quad (42)$$

$$\int_{0}^{E_M} f(E,0)(<E> - E)^2 dE = F^{-1} \left[ \int_{0}^{E_M} f(E,0)(E_M - E)dE \right]^2, \quad (43)$$

The distribution of reduced energy densities, \(E_{<E>}\), is defined by the probability density function

$$f_r\left(\frac{E}{<E>} t\right), \quad (44)$$

with

$$f_r\left(\frac{E}{<E>} t\right) = <E> f(E,t) = <E> > F^{-1} f(E,0). \quad (45)$$

In the following section we apply these results to power law distributions of the energy density, for which, as we shall see, grain growth leads to a scaling regime.

### 3.1.2. Power law energy distributions

These distributions are defined by probability density functions of the type

$$f(E,0) = \alpha E^{\alpha - 1}; 0 \leq E \leq 1; \alpha > 0, \quad (46)$$

where \((\alpha - 1)\) is the power law exponent \((\alpha > 0)\). For \(\alpha = 1\) all energy densities are equiprobable. The factor \(F\) is (eq. (31))

$$F = E_M^\alpha. \quad (47)$$

Eq. (34) defining \(E_M(t)\) becomes

$$n!\alpha! E_M^{(\alpha - 1)n} = 1; t > t_1. \quad (48)$$

The maximum energy density, \(E_M\), has a power law decrease with time. The time, \(t_1\), at which the first grain \((E_M = 1)\) disappears is

$$t_1 = \left[ \frac{(n + \alpha)!}{n!\alpha!} \right]^{1/n}. \quad (49)$$

For the time dependence of \(<a>\) we obtain from eq. (38)

$$<a> = \frac{E_M}{\alpha + 1}. \quad (50)$$

Eliminating \(E_M\) between eqs. (46) and (48) yields

$$<a> = \frac{1}{\alpha + 1} \left[ \frac{(n + \alpha)!}{n!\alpha!} \right]^{\frac{1}{n+\alpha}} t, \quad (51)$$

with

$$\mu = \frac{\alpha}{\alpha + n}. \quad (52)$$

The average grain diameter has a power law increase with time, with a positive exponent

$$\frac{dE}{dt} = \frac{\alpha}{\alpha + n} E^\mu. \quad (53)$$
\[ \mu = \frac{\alpha}{\alpha + n} \] smaller than 1, which increases with \( \alpha \). For a uniform energy distribution (\( \alpha = 1 \)), the exponent is 1/3 in 2D and 1/4 in 3D. The value of \( \alpha \) for which the kinetics are parabolic (\( < a > \propto t^{1/2} \)) is \( \alpha = n \). It is also possible to obtain, respectively from eqs. (35) and (36)

\[
E^* = \frac{\alpha}{\alpha + n} E_M, \quad (50a)
\]

\[
< E > = \frac{\alpha}{\alpha + 1} E_M. \quad (50b)
\]

The ratios \( E^*/< E > \) and \( E_M/< E > \) are therefore time independent. Note that \( E^*/E_M \) is the exponent of the power law (eq. (49a)) for \( < a > (t) \). The variance of the diameter distribution is also a constant

\[
s^2 = \frac{\alpha}{\alpha + 2} \quad (51)
\]

and increases as \( \alpha \) increases.

We finally turn to the distributions of grain diameter. The distribution of \( a \) is defined by (from eqs. (40), (29) and (45))

\[
g(a,t) = \frac{\alpha}{E_M t} \left( 1 - \frac{a}{E_M t} \right)^{-\alpha - 1}, \quad (52)
\]

with \( E_M (t) \) given by eq. (46). The distribution of reduced diameters is

\[
g_r \left( \frac{a}{< a >} \right) = \frac{\alpha}{\alpha + 1} \left( 1 - \frac{a}{E_M t} \right)^{-\alpha - 1}. \quad (53)
\]

Combining eq. (53) with eq. (48) to eliminate \( E_M(t) \) we finally obtain

\[
g_r \left( \frac{a}{< a >} \right) = \frac{\alpha}{\alpha + 1} \left[ 1 - \frac{1}{\alpha + 1} \frac{a}{< a >} \right]^{-\alpha - 1} \quad (54)
\]

which is time independent. There is a scaling regime with a distribution independent of \( n \). It is easily shown that \( g_r \) is normalized to one and has unit average value. To show this, it is enough to note that the largest \( a \) at time \( t \) is \( a_0 (t) = E_M t; \) from eq. (48) it follows that \( \frac{a}{< a >} \) is in the interval \([0, \alpha + 1]\).

### 3.2. Non-uniform initial grain size

The previous analysis considered uniform grains in the initial state, \( a_E(0) = 1 \). The grains disappear in the order of decreasing energy density. We will show that the analysis can also be applied to arbitrary initial distributions of grain sizes.

Consider first the case where the sequence of grain elimination is that of decreasing energy, but the initial diameters are not uniform. This can happen if the initial diameters are defined by a non-increasing function \( a(E,0) = a_E(0) \) such that the grains again disappear in the order of decreasing \( E \). Integration of eq. (26) then gives

\[
a_E(t) - a_0(t) = \phi(E) - E t, \quad (55)
\]

where

\[
\phi(E) = a_E(0) - a_0(0); \quad (\phi(E)\leq 0). \quad (56)
\]

The maximum energy at time \( t \), \( E_M(t) \), is given by

\[
E_M t = \phi(E_M) + a_0(t) \quad (57)
\]

and the diameter \( a_E \) of a grain with energy \( E \) at time \( t \) is

\[
a_E(t) = \phi(E) - \phi(E_M) + (E_M - E) t, \quad (58)
\]

which generalizes eq. (28). The equations for \( E_M(t) \) and \( < a > (t) \) (eqs. (34) and (37)) are correspondingly altered. But at large \( t \), the first term on the right-hand side of eq. (57) can be neglected and the equation reduces to eq. (29). All equations derived in Section 3.1 therefore apply at sufficiently long times, when the sequence of grain elimination is that of decreasing energy density.

In the more general case when the initial grain diameters and energies are such that grains of smaller energy may disappear before grains of larger energy, the polycrystal evolves to a state, at sufficiently long times, in which the order of increasing diameters is the order of decreasing energy density. Consider in fact, two grains \( 1 \) and \( 2 \) with \( E_2 > E_1 > E^* \) and \( a_2 > a_1 \). Since the rate of growth is proportional to \( E^* - E \), grain 2 shrinks faster than grain 1 and will eventually become smaller than grain 1. If \( E^* > E_2 > E_1 \) with \( a_2 > a_1 \), both grains grow but since 1 grows faster it will eventually become larger than grain 2. At long
times, the order of increasing diameter is that of decreasing energy.

In conclusion, after a transient the equations derived in Section 3.1 apply. In particular, a scaling regime will be reached for power law energy density distributions irrespective of the initial grain diameter distribution. When the initial diameters are uniform, scaling is reached just after elimination of the first grain; otherwise there will be a transient before the scaling regime is reached. We have checked these conclusions by numerical integration of the growth equation (see Section 4).

### 3.3. Other energy distributions: condition for scaling

The general equations of Section 3.1 can be applied to any initial energy and diameter distributions. However, a scaling regime will in general not be reached and the kinetics will be ever changing. The necessary condition for scaling is that the distribution of the reduced diameters, 

$$g_r(a/a_0, t),$$

is time independent, at least at long times. Using eqs. (29) and (39) we may write

$$g_r(a/a_0, t) = \frac{E_M - E}{E_M - E_r}.$$  \hspace{1cm} (59)

Introducing eq. (39) in eq. (40) and using eq. (43), the probability density function 

$$g_r(a/a_0)$$

becomes

$$g_r(a/a_0) = (E_M - E_r) I^{-1}(E, 0)$$ \hspace{1cm} (60)

$$= \left( \frac{E}{E_r} - 1 \right) I^{-1}(E, 0).$$

We wish to determine the initial energy distributions \(f(E, 0)\) such that \(g_r\), given by eq. (60) is time independent. As shown in Section 3.1.2, this happens when \(f(E, 0)\) is a power function of exponent larger than \((-1)\). And there are no other \(f(E, 0)\) that satisfy the scaling condition, as the following simple argument shows. In a scaling regime, the distribution of reduced energy densities \(E/\langle E\rangle\) must be time invariant; in particular \(E_M/\langle E\rangle\) must be a constant. It is easily shown that this condition is met if and only if \(f(E, 0)\) has a power dependence on \(E\). Consider, for example, a distribution \(f(E, 0)\) in the form of a sum of various powers of \(E\); \(E_M/\langle E\rangle\) is not time invariant and thus a scaling regime is not reached. It can be shown that at long times the kinetics \(\langle a/a_0 \rangle(t)\) are governed in this case by the smaller power exponent in \(f(E, 0)\). This follows from eqs. (34) and (38). We have checked this conclusion with the computer simulations described in the following section (see Fig. 2a).

### 4. Numerical simulations

Numerical calculations were undertaken to investigate the mixed effect of curvature and energy density differences in grain growth. We also studied numerically the “pure” cases: pure energy driven growth and pure curvature driven growth, in order to more easily compare these with the mixed case and also to validate the numerical code. All simulations were made for 2D polycrystals because the 2D steady state distributions under pure curvature growth are known [3]. The initial number of grains was 10 000. Essentially, we applied the relevant growth equation to follow the time evolution of each individual grain (i.e., its diameter). This requires the determination of the thresholds \(E^*\) and \(a^*\) at each time, which is achieved by an explicit iteration scheme involving these thresholds and the updated values of the diameters. At each time step, typically three or four iterations are needed to stabilize the values of the thresholds. At the end of the simulations (around 1000 surviving grains), the total area of the grains was calculated and compared to the initial area, to assess the accuracy of the calculations. The differences were in all cases below 3%.

The initial grain diameter distributions used (with \(\langle a \rangle = 1\)) were of the following types:

1. Uniform grain size (except for pure curvature).
2. Quasi-uniform grain size (for pure curvature and mixed effects) with the initial grain diameters uniformly distributed in the interval \(± 10^{-4}\).
3. Hillert’s stationary distribution [1]. This distribution is defined by
Fig. 1. Computer calculations of the evolution of the diameter distribution in (pure) curvature driven 2D grain growth for three initial diameter distributions: a) Hillert’s distribution; b) quasi-uniform grain size; c) Rayleigh distribution. d) The time variation of the kinetic exponent $\mu$ and e) the time variation of the variance $s^2$, for the three diameter distributions.

4. Rayleigh distribution. This distribution is defined by

$$g_r(u,0) = \frac{\pi}{2} u \exp\left(-\frac{\pi}{2} u^2\right); \quad u = \frac{a}{<a>};$$

and is a particular form of the gamma distribution function. In the computations, the distribution was truncated at $u = 3.5$.

The initial energy distributions (energies in $[0,1]$) that were combined with the diameter distributions were simple power laws of the type of eq. (44) with $\alpha = 1$ (uniform distribution), $\alpha = 2$ (which for the pure energy case leads to parabolic growth) and $\alpha = 3$; and a linear combination of $\alpha = 1$ and $\alpha = 3$ power laws.
Fig. 2. The time variation (full lines) of: (a) the average grain diameter \( <a> \), and b) the variance \( s^2 \) of the diameters obtained by computer calculation of 2D grain growth driven by (pure) energy density differences, \( E \). The initial \( E \) distribution is a one-one linear combination of power distributions of exponents \( \alpha = 1 \) and \( \alpha = 3 \). The straight lines (dashed) are for the scaling regimes with separate \( \alpha = 1 \) and \( \alpha = 3 \).

The diameter distribution and the energy density distribution were combined in various ways to define the initial state. Three types of correlations were used: a) random, in which the energy \( E \) of a grain of diameter \( a \) was randomly taken from the \( E \) distribution; b) “increasing”, with \( E \) increasing with \( a \); c) “decreasing”, with \( E \) decreasing with \( a \).

Finally, we also studied the effect of the initial value of the parameter \( R = k'/(k <a> <E>) \) previously defined (eq. (20)), which measures the relative weight of curvature and energy density effects on grain growth. This was achieved by changing \( k'/k \).

In addition to the global kinetics, \( <a> (t) \), we determined in each simulation the evolution of the distributions of the reduced diameters \( g_b(a / <a>) \) and the variance \( s^2 \). We made no attempt at obtaining the compound distributions \( h_b(a,E,t) \) and \( h(a,<a>,E,<E>,t) \). We describe separately the results obtained for the three groups of simulations (pure curvature, pure energy and mixed effects). Tables 1–3 contain a compilation of the results, obtained in the simulations, of the kinetic exponent \( \mu \) in the relation \( <a> \propto t^{\mu} \) and of the standard variance \( s^2 \) of the diameter distribution, for the various cases studied. The values given in the tables are those reached at long times, when the number of surviving grains is around 1000.

4.1. Pure curvature

As could be anticipated, Hillert’s distribution was unchanged by growth (Fig. 1a) and the kinetics were parabolic. The other two (quasi-uniform grains and Rayleigh distribution) evolved to what can be taken as a quasi-stationary regime. The evolution of the two distributions is shown in Fig. 1b and c, respectively. They approximately fit in the one parameter, \( \nu \), family of steady state distributions identified by Rios [3], with \( \nu = 5.25 \) (quasi-uniform initial distribution) and \( \nu = 3.0 \) (Rayleigh initial distribution). The kinetic exponent \( \mu \) and the variance \( s^2 \) for the three distributions studied are shown as a function of \( t \) in Fig. 1d and e, respectively. Table 1 contains a compilation of the results obtained for \( \mu \) and \( s^2 \) at the end of the simulations (~1000 grains left). Note that the kinetic exponent \( \mu = 1/2 \) is only reached for the scaling Hillert’s distribution.

<table>
<thead>
<tr>
<th>Table 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Long time parameters in pure curvature growth</td>
</tr>
<tr>
<td>Initial diameter distribution</td>
</tr>
<tr>
<td>Quasi-uniform</td>
</tr>
<tr>
<td>Hillert</td>
</tr>
<tr>
<td>Rayleigh</td>
</tr>
</tbody>
</table>

\( \mu \) = Power law kinetic exponent.
\( s^2 \) = Variance of diameter distribution.
Table 2
Mixed curvature/energy growth: effect of initial diameter distribution and energy density distribution on long time parameters (R=1; “decreasing” correlation)

<table>
<thead>
<tr>
<th>Initial diameter distribution</th>
<th>α=1</th>
<th>α=2</th>
<th>α=3</th>
<th>Pure curvature</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>µ</td>
<td>s²</td>
<td>µ</td>
<td>s²</td>
</tr>
<tr>
<td>Quasi-uniform</td>
<td>0.44</td>
<td>0.10</td>
<td>0.50</td>
<td>0.19</td>
</tr>
<tr>
<td>Hillert</td>
<td>0.44</td>
<td>0.11</td>
<td>0.50</td>
<td>0.19</td>
</tr>
<tr>
<td>Rayleigh</td>
<td>0.43</td>
<td>0.13</td>
<td>0.48</td>
<td>0.20</td>
</tr>
<tr>
<td>Pure energy</td>
<td>0.33</td>
<td>0.33</td>
<td>0.50</td>
<td>0.50</td>
</tr>
</tbody>
</table>

µ = Power law kinetic exponent.
s² = Variance of diameter distribution.

Table 3
Mixed curvature/energy growth: effect of R and initial correlation on long time parameters (Hillert initial diameter distribution; α = 1)

<table>
<thead>
<tr>
<th>Correlation</th>
<th>Random correlation</th>
<th>Decreasing correlation</th>
<th>Increasing correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>µ</td>
<td>s²</td>
<td>µ</td>
</tr>
<tr>
<td>Pure energy</td>
<td>0.33</td>
<td>0.33</td>
<td></td>
</tr>
<tr>
<td>(α=1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R = 1/9</td>
<td>0.38</td>
<td>0.17</td>
<td>0.38</td>
</tr>
<tr>
<td>R = 1</td>
<td>0.44</td>
<td>0.13</td>
<td>0.44</td>
</tr>
<tr>
<td>R = 9</td>
<td>0.50</td>
<td>0.13</td>
<td>0.49</td>
</tr>
<tr>
<td>Pure curvature</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

µ = Power law kinetic exponent.
s² = Variance of diameter distribution.

4.2. Pure energy

The simulations for the simple power laws confirmed the predictions of the theoretical analysis of Section 3.2. Scaling is clearly reached, with a power law distribution of diameters and a kinetic law <a> (t) as predicted (eq. (49)). The steady state distributions are independent of the initial diameter distribution and of the initial correlation between size and energy. We also simulated the evolution under an energy distribution consisting of a linear combination, with coefficients 1, of power laws for α = 1 and α = 3. The kinetics are intermediate between those for α = 1 and α = 3 and evolves as predicted, as is shown by the <a> (t) and s²(t) curves of Fig. 2 for initial uniform grain diameters. Scaling is not reached. Similar results were obtained for a Hillert initial distribution.

4.3. Mixed effects

In most simulations we used R = 1 (eq. (20)) and studied separately the effect of R. When curvature is mixed with a power law energy distribution of exponent (α−1) the distributions at long times evolve slowly, indicating that a scaling regime is not reached. The distributions and the values of s²
and $\mu$ that we indicate are those reached at long times, when the number of grains is reduced to ~1000.

### 4.3.1. Effect of initial diameter distribution

Table 2 shows the effect of varying the initial distribution on the kinetic exponent $\mu$ and on the variance $s^2$ at long times for $R = 1$ and the "decreasing" combination of $\alpha$ and $E$, and for $\alpha = 1$, $\alpha = 2$ and $\alpha = 3$. The values of $\mu$ and $s^2$ for pure curvature growth (Table 1) and for pure energy are included for comparison. The distributions at long times deviate in all cases from those obtained under pure curvature or pure energy, as expected.

The kinetic exponents $\mu$ are intermediate between those for pure curvature and pure energy (with the same $\alpha$). For $\alpha = 2$, the kinetic exponent is $1/2$ and is reached in two simulations. However, the variances differ from those for the pure cases, reflecting a change in the long time distributions. We give two examples of this change in Fig. 3 which applies to an initial Hillert distribution (this distribution remains unchanged in pure curvature growth) and to initial quasi-uniform grain sizes.

### 4.3.2. Effect of power law exponent $\alpha$ of energy distribution

The data in Table 2 illustrates the effect of $\alpha$. Increasing $\alpha$ increases the kinetic exponent $\mu$ and the variance $s^2$.

### 4.3.3. Effect of initial combination of $\alpha$ and $E$

Table 3 shows results obtained, for fixed $R$, for different combinations of an initial Hillert distribution of diameters and a uniform energy distribution ($\alpha = 1$). The kinetic exponent $\mu$ is little affected but $s^2$ is larger for the "random" combination.

### 4.3.4. Effect of relative weight ($R$) of curvature and energy

The effect of $R$ is illustrated in Table 3, for the Hillert initial diameter distribution. The parameter $R$ affects both $\mu$ and $s^2$. As expected, increasing $R$ accelerates the kinetics, since the exponent is $\mu = 1/2$ for pure curvature and $\mu = 1/3$ for pure energy, with $\alpha = 1$.

### 5. Conclusion

A generalized theoretical framework was described, enabling incorporation in the same formalism of grain growth that is driven either by curvature or by an external driving force or by both.

The mean field approach that was used leads to the definition of a threshold energy, $E^*$, which is a weighted average of the energy densities of the individual grains. This threshold energy density
defines which grains grow and shrink at any time and the respective rate.

The growth equation for negligible curvature effect can be handled analytically, leading to a general kinetic relation between average grain diameter and time and to an evolutionary equation for the grain diameter distribution. When the energy density has a power law distribution, a scaling regime with a definite power law kinetics is reached, which is independent of the initial distribution of grain diameters.

For curvature driven growth superimposed on energy density differences, the growth equations were solved numerically. The simulations seem to indicate that a scaling regime is in general not reached under the combined effects of curvature and energy, even when energy alone leads to scaling. The resulting kinetics are defined by a power law with a (non-constant) exponent intermediate between those for pure curvature ($\mu = 1/2$) and pure energy. The quasi-steady state diameter distributions reached at long times depend on the initial distributions and on the way they are combined. The exponent $\mu$ in the global power law kinetics, however, seems to be independent of these two factors, while being determined by the weighing parameter, $R$, and by the exponent of the power law energy distributions.

The results that were obtained provide a guide to the control of grain growth by applied fields with the purpose of favoring grain orientations of low energy density and therefore controlling the grain crystallographic texture. The relevant parameter in this context is the width of the energy density distribution, which can be easily obtained from the simulations.

References