A probabilistic model for predicting grain growth processes in alloys

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Abstract. This paper deals with a possible generalization of the traditional grain growth kinetic functions. A novel probabilistic model devoted to the grain growth prediction in alloys is presented. It is based on the extension of the traditional power law kinetic equation proposed by Beck. The Beck’s isothermal kinetic equation is defined as \( D(t) = A \cdot \exp\left(-\frac{E}{RT}\right) \cdot t^m \) where \( D(t) \) is the grain size (diameter), \( t \) is the time, \( E \) is the activation energy, \( A \) is the preexponential factor, \( m \) is the time exponent, \( R \) is the universal gas constant and \( T \) is the absolute temperature. The novel probabilistic model proposed is based on the concept of the mixture of probability density functions. In this model it is assumed that during grain growth the activation energy (\( E \)) is not constant, but its distribution is determined by the initial grain morphology of alloys. More exactly speaking, it is supposed that the activation energy is a random variable which is characterized by the probability density function \( g(E) \) of the activation energy. By using appropriately selected probability density functions, different types of generalized grain growth kinetic equations can be established. Based on computer simulations, the application of the extended grain growth kinetic models is demonstrated by examples.

1. Introduction
The traditional isothermal kinetic function of the isothermal grain growth process [1, 2] is represented by the equation:

\[
D(t,T,E) = K(T,E) t^m = Ae^{\left(\frac{E}{RT}\right)}t^m
\]

where \( D(t) \) is the grain size (diameter), \( t \) is the time, \( E \) is the activation energy in J/mol, \( A \) is the preexponential factor, \( m \) is the time exponent, \( R \) is the universal gas constant (\( R=8,314 \) J/mol) and \( T \) is the absolute temperature of transformation in degree Kelvin. In the above equation:

\[
K = K(T,E) = Ae^{\left(\frac{E}{RT}\right)}
\]

is the Arrhenius formula describing the temperature dependence in the kinetic function.
During last three decades, the grain growth kinetics have been extensively studied and several attempts have been made [3-6] for extending the above kinetic equation in order to improve its prediction accuracy.

In what follows, a novel probabilistic concept is outlined in which it is assumed that activation energy is not constant, but it is determined primarily by the local microstructure of alloys subjected to heat treatment.

2. Construction of novel grain growth kinetic functions using a probabilistic concept

In the generalized kinetic model proposed it is assumed that in the grain growth process, the activation energy \( E \) is not constant, but it is determined by the initial microstructure. More exactly speaking, we assume that the activation energy is a random variable and its distribution is unambiguously characterized by a continuous probability density function \( g(E) \).

Construction of generalized grain growth kinetic functions of novel type is based on the concept of the mixture of probability distribution functions [7].

Staring with the hypothesis outlined above the extended version of the novel grain growth kinetic equation can be described in the following general form:

\[
D(t, g) = \int_{0}^{\infty} D(t, T, E) g(E) dE = A t \int_{0}^{\infty} e^{-\left(\frac{E}{RT}\right)} g(E) dE
\]

As we have already mentioned in the above equation the activation energy is supposed to be a continuous random variable. The probability density function \( g(E) \) describing the change of non-constant activation energy \( E \) can be selected in various ways. In what follows, three different versions of the proposed probabilistic model are outlined.

**Model 1** Let us assume that the activation energy is considered as a random variable \( E_b \), and it is characterized by the following uniform probability density function

\[
g_u(E) = \frac{1}{E_2 - E_1}
\]

where \( E_2 > E_1 \geq 0 \). The corresponding generalized kinetic equation will be

\[
D(t, g_u) = \int_{E_i}^{E_2} D(t, T, E) g_u(E) dE = A t \int_{E_i}^{E_2} e^{-\left(\frac{E}{RT}\right)} \frac{1}{E_2 - E_1} dE
\]

Because for \( b=1/(RT) \)

\[
\int_{E_i}^{E_2} e^{-bE} dE = \frac{1}{b} \left( e^{-bE_i} - e^{-bE_2} \right) = RT \left\{ e^{\frac{E_i}{RT}} - e^{\frac{E_1}{RT}} \right\}
\]

this implies that

\[
D(t, g_u) = \frac{A t}{E_2 - E_1} \int_{E_i}^{E_2} e^{-\left(\frac{E}{RT}\right)} dE = \frac{A R T t}{E_2 - E_1} \left\{ e^{\frac{E_i}{RT}} - e^{\frac{E_2}{RT}} \right\}
\]
It is easy to see that the above equation can be rewritten in following form:

$$D(t,g_U) = \frac{RT^m}{E_2 - E_1} \left\{ \exp \left( \frac{E_1}{RT} \right) - \exp \left( \frac{E_2}{RT} \right) \right\} = \frac{RT^m}{E_2 - E_1} \left\{ K(T, E_1) - K(T, E_2) \right\}.$$ 

It is clear that because the activation energy is a random variable (denoted by $E_\varphi$), consequently, according to the Arrhenius formula, $K_\varphi$ is also considered as a random variable given as function of $E_\varphi$.

Based on the relation between the random variables $E_\varphi$ and $K_\varphi$, we can generate the probability density function $f(K, g_U)$ of $K_\varphi$ in the following form:

$$f(K, g_U) = \frac{RT}{K(E_2 - E_1)}$$

The corresponding probability density functions of random variables $E_\varphi$ and $K_\varphi$ are depicted in Figure 1.

**Figure 1.** The probability density functions of random variables $E_\varphi$ and $K_\varphi$.

**Model 2** Let us assume that the random variable $E_\varphi$ is characterized by the following probability density function

$$g_R(E) = \frac{1}{RT \left\{ \exp \left( -\frac{E_1}{RT} \right) - \exp \left( -\frac{E_2}{RT} \right) \right\} \exp \left( -\frac{E}{RT} \right) = C \exp \left( -\frac{E}{RT} \right)}$$

(5)
where $E_2 > E_1 \geq 0$, and

$$
C = RT \left\{ \exp \left( - \frac{E_1}{RT} \right) - \exp \left( - \frac{E_2}{RT} \right) \right\} = \frac{RT}{A} \{ K(T,E_1) - K(T,E_2) \} = \frac{RT}{A} \{ K_1 - K_2 \}
$$

is a positive constant, by definition.

For the corresponding generalized kinetic function one obtains that

$$
D(t,g_B) = At^m \int_{E_1}^{E_2} e^{-\left( \frac{E}{RT} \right)} g_B(E) dE = \frac{At^m E_2}{C} \int_{E_1}^{E_2} \left( e^{-\left( \frac{E}{RT} \right)} \right)^2 dE
$$

By introducing the novel variable defined by

$$
u(E) = \exp \left( - \frac{E}{RT} \right)
$$

as a result of transformation we have

$$
\int_{E_1}^{E_2} \left( e^{-\left( \frac{E}{RT} \right)} \right)^2 dE = -RT \int_{u(E_1)}^{u(E_2)} u^2 \frac{1}{u} du = RT \int_{u(E_1)}^{u(E_2)} ud(u) = \frac{RT}{2} \left\{ \left( e^{-\left( \frac{E_1}{RT} \right)} \right)^2 - \left( e^{-\left( \frac{E_2}{RT} \right)} \right)^2 \right\}.
$$

From the above identity it follows that

$$
D(t,g_B) = \frac{At^m E_2}{C} \int_{E_1}^{E_2} \left( e^{-\left( \frac{E}{RT} \right)} \right)^2 dE = At^m \left( \frac{RT}{2} \right) \frac{\left\{ \left( e^{-\left( \frac{E_1}{RT} \right)} \right)^2 - \left( e^{-\left( \frac{E_2}{RT} \right)} \right)^2 \right\}}{RT \left\{ \exp \left( - \frac{E_1}{RT} \right) - \exp \left( - \frac{E_2}{RT} \right) \right\}}
$$

Finally we get

$$
D(t,g_B) = \frac{At^m}{2} \left\{ \exp \left( - \frac{E_1}{RT} \right) + \exp \left( - \frac{E_2}{RT} \right) \right\} = \frac{t^m}{2} \{ K_1 + K_2 \}.
$$

From the previous considerations we can conclude that the density function of $K_B$ is

$$
f(K_B) = \frac{1}{K_2 - K_1}
$$

which represents the traditional uniform probability density function.

The corresponding probability density functions of random variables $E_B$ and $K_B$ are depicted in Figure 2.
Model 3 Let us assume that the random variable $E_\vartheta$ is characterized by the following exponential probability density function

$$g_E(E) = \lambda e^{-\lambda (E-E_0)}$$

(6)

where $E > E_0 \geq 0$ and $\lambda > 0$.

In this case the generalized grain growth kinetic equation will be:

$$D(t, g_E) = \int D(t, T, E) g_E(E) dE = A t^m \int_{E_0}^{\infty} e^{\frac{-E}{RT}} \left[ \lambda e^{-\lambda (E-E_0)} \right] dE.$$

Figure 2. The probability density functions of random variables $E_\vartheta$ and $K_\vartheta$.

By introducing the new variable $u = E - E_0$, and performing the corresponding transformation, one obtains that

$$D(t, g_E) = \lambda A t^m e^{-\lambda E_0} \int_{0}^{\infty} e^{\frac{-u}{RT} + \lambda u} du.$$

For any number $a > 0$, 

$$D(t, g_E) = \lambda A t^m e^{-\lambda E_0} \int_{0}^{\infty} e^{\frac{-u}{RT} + \lambda u} du.$$
holds. Consequently, by selecting \( a = \lambda + 1/(RT) \), one obtains that

\[
D(t, g_E) = \lambda A t^m \exp \left( \frac{E_0}{RT} \right) \int_0^\infty e^{-\left( \frac{1}{(RT)^{+\lambda}} \right) \mu} d\mu = \lambda A e^{-\left( \frac{E_0}{RT} \right)} \left( \frac{RT}{1 + \lambda RT} \right)^m t^m.
\] (7)

3. Computer simulation of austenite grain growth

In what follows some computational results are presented. Based on the computer simulation of grain growth process, the results obtained by the traditional and the generalized kinetic equations are compared and discussed.

3.1 Predicting the grain growth process using the traditional isothermal kinetic model

Computations for simulating the isothermal grain growth process using the traditional kinetic model (represented equation (1)) were performed with the following parameter set: \( A = 76000 \), \( E = 70000 \text{ J/mol} \), \( m = 0.2 \).

For temperatures \( T = 1173 \text{ °K} \) and \( T = 1273 \text{ °K} \), the change of computed grain size (\( D \)) as function of time (\( t \)) is depicted in Figure 3.

3.2 Predicting the grain growth process supposing a changing activation energy

For testing the generalized grain growth model characterized by the changing activation energy, we used the probability density function defined by equation (6):

\[
g_E(E) = \lambda e^{-\lambda(E-E_0)}
\]

where \( E > E_0 \geq 0 \) and \( \lambda > 0 \).
In this case, the corresponding generalized grain growth kinetic function is given as:

$$D(t, g_E) = \lambda At^m e^{\frac{E_0}{RT}} \int_0^\infty e^{\frac{1}{RT} + \lambda u} du = \lambda Ae^{\frac{E_0}{RT}} \left\{ \frac{RT}{1 + \lambda RT} \right\} t^m.$$  

It is easy to see that the above kinetic function can be rewritten in the following simplified form:

$$D(t, g_E) = C(\lambda, T) * C(E_0, T) * At^m$$

where

$$C(\lambda, T) = \frac{\lambda RT}{1 + \lambda RT}$$

and

$$C(E_0, T) = e^{\frac{E_0}{RT}}.$$  

The model parameters were selected as follows: $E_0 = 70000$ J/mol, $\lambda = 1/10000$, $A = 76000$, $m = 0.2$.

i) For temperature $T = 1173$ °K, the generalized grain growth function can be formulated as

$$D(t, g_E) = C(\lambda, T) * C(E_0, T) * At^m$$

where

$$C(\lambda, T) = \frac{\lambda RT}{1 + \lambda RT} = \frac{0.0001 \times 8,314 \times 1173}{1 + 0.0001 \times 8,314 \times 1173} = 0.49373$$

and

$$C(E_0, T) = e^{\frac{E_0}{RT}} = e^{\frac{70000}{8,314 \times 1173}} = 0.000763.$$

ii) For temperature $T = 1273$ °K, the generalized grain growth kinetic function will be

$$D(t, g_E) = C(\lambda, T) * C(E_0, T) * At^m$$

where

$$C(\lambda, T) = \frac{\lambda RT}{1 + \lambda RT} = \frac{0.0001 \times 8,314 \times 1273}{1 + 0.0001 \times 8,314 \times 1273} = 0.514179$$

and
For temperatures $T=1173\,^{\circ}\!\!K$ and $T=1273\,^{\circ}\!\!K$, the change of computed grain size ($D$) as function of time ($t$) is depicted in Figure 4.

\[
C(E_0, T) = e^{\left(\frac{E_0}{RT}\right)} = e^{\left(\frac{70000}{8.314\times1273}\right)} = 0.0013415
\]

\[
E > E_0 = 70000\, \text{J/mol}
\]

\[
T = 1000\,^{\circ}\!\!C
\]

\[
T = 900\,^{\circ}\!\!C
\]

**Figure 4.** Predicted austenite grain size at temperatures $T=900\,^{\circ}\!\!C$ and $T=1000\,^{\circ}\!\!C$.

### 4. The influence of the initial (deformed) microstructure on the grain growth kinetics

A general observation is that the initial microstructure of alloys has a significant effect on the progress of grain growth processes. The kinetics of recrystallization is strongly influenced by the stored energy of deformed grains [8-10]. The stored energy in individual grains depends considerably on the degree of cold deformation. This means that the stored energy distribution in grains (the activation energy for the recrystallization) is determined by the deformation distribution in grains.

**Figure 5.** Geometric models of single-phase polyhedral microstructures: Original microstructure (A), microstructure obtained by a plastic tensile deformation (B), microstructure obtained by a plastic compressive deformation (C).

Due to non-uniform deformation degree distribution, the morphology (shape) of each individual grain will be distinct. The influence of non-uniform deformation distribution on the change of grain geometry is illustrated by the following simple model. Figure 5 shows three idealized single-phase
microstructures before and after cold deformations. A common feature of three model microstructures denoted by A, B and C is that they are composed of 8 congruent parallelepipeds representing the individual grains.

Based on the von Mises criterion, the total effective plastic strain can be calculated by:

$$\varepsilon_{tp} = \sqrt{\frac{2}{3}(\varepsilon_{1p}^2 + \varepsilon_{2p}^2 + \varepsilon_{3p}^2)}$$

where $\varepsilon_{1p}$, $\varepsilon_{2p}$ and $\varepsilon_{3p}$ are principal plastic strains [11, 12].

Because $\ln(1/2) = -0.693$, $\ln(2) = 0.693$, $\ln(4) = 1.386$ and $\ln(1/4) = -1.386$, it is easy to check that for deformed microstructures B and C the computed total effective plastic strains are equal:

$$\varepsilon_{tp}(B) = \sqrt{\frac{2}{3}(\varepsilon_{1p}^2 + \varepsilon_{2p}^2 + \varepsilon_{3p}^2)} = \sqrt{\frac{2}{3}[-0.692]^2 + (1.386)^2 + (-0.692)^2} = 1.38629$$

and

$$\varepsilon_{tp}(C) = \sqrt{\frac{2}{3}(\varepsilon_{1p}^2 + \varepsilon_{2p}^2 + \varepsilon_{3p}^2)} = \sqrt{\frac{2}{3}[(0.692)^2 + (0.692)^2 + (-1.386)^2]} = 1.38629$$

However, comparing the geometry of grains, we can observe that their volume is equal ($V = a^3/8$) in all cases, but the surface area $S$ of the individual grains is different. For grains included in microstructures A, B and C, we get $S(A) = 1.5a^2$, $S(B) = 2.125a^2$ and $S(C) = 2.5a^2$, respectively.

From this observation we can conclude that although the deformation degree is identical for microstructures B and C, however it is expected that the recrystallization rate in microstructure C will be faster than in microstructure B, due to the larger specific surface area of deformed grains.

5. Another possible generalization of kinetic models of grain growth processes

The probabilistic kinetic model proposed for predicting the grain growth processes can be easily extended on the basis of the following concept. Starting with the classical grain growth kinetic equation represented by

$$D(t) = Ae^{-(E_{RT})t^m}$$

define the following 3 uniform probability density functions of parameters $A$, $E$ and $m$ as follows:

$$\text{gu}(A) = \frac{1}{A_2 - A_1} \quad \text{where } A_2 > A_1 \geq 0,$$

$$\text{gu}(E) = \frac{1}{E_2 - E_1} \quad \text{where } E_2 > E_1 \geq 0,$$

$$\text{gu}(m) = \frac{1}{m_2 - m_1} \quad \text{where } m_2 > m_1 \geq 0.$$
D(t, gu(A), gu(E), gu(m)) = \frac{1}{h(A, E, m)} \left( \int_{A_1}^{A_2} A dA \int_{E_1}^{E_2} e^{\frac{E}{RT}} dE \int_{m_1}^{m_2} t^m dm \right)

where

h(A, E, m) = (A_2 - A_1)(E_2 - E_1)(m_2 - m_1)

and

\int_{A_1}^{A_2} A dA = \frac{(A_2^2 - A_1^2)}{2}

\int_{E_1}^{E_2} e^{\frac{E}{RT}} dE = RT \left( e^{\frac{E_2}{RT}} - e^{\frac{E_1}{RT}} \right)

\int_{m_1}^{m_2} t^m dm = \frac{1}{\ln t} \left( t^{m_2} - t^{m_1} \right).