

Real and extended volumes in simultaneous transformations

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The relationship between real and extended volumes is expanded to an indefinite number of simultaneous transformation processes. The assumption used in the present study is that the growth and nucleation of each product phase occurs randomly throughout the transforming region. The real volume of each phase is given in the form of an integral, using the extended volumes. Once the extended volumes of different product phases are related, the real volume of each product phase can be analytically or numerically calculated, and analytical solutions for cases where the extended volumes are related linearly or parabolically are given.

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Introduction

A model for a single transformation begins with the calculation of the nucleation and growth rates using classical theory,¹⁻⁶ but an estimation of the volume fraction requires impingement between particles to be taken into account. This is generally achieved using the extended volume concept of Kolmogorov, Johnson and Mehl, and Avrami (details are given in Ref. 1) as illustrated in Fig. 1. Suppose that two particles exist at time t : a small interval δt later, new regions marked a, b, c, and d are formed assuming that they are able to grow unrestricted in extended space whether or not the region into which they grow is already transformed. However, only those components of a, b, c, and d which lie in previously untransformed matrix can contribute to a change in the real volume of the product phase (identified by the subscript 1)

$$dV_1 = \left(1 - \frac{V_1}{V}\right) dV_1^e \quad \dots \quad (1)$$

where it is assumed that the microstructure develops randomly. The superscript e refers to extended volume, V_1 is the volume of phase 1, and V is the total volume. Multiplying the change in extended volume by the probability of finding untransformed regions has the effect of excluding regions such as b, which clearly cannot contribute to the real change in volume of the product. This equation can readily be integrated to obtain the real volume fraction

$$\frac{V_1}{V} = 1 - \exp\left(-\frac{V_1^e}{V}\right) \quad \dots \quad (2)$$

In practice, there are many instances where several transformations occur together. The different reactions interfere with each other in a manner which is fundamental to the development of many steel microstructures. Therefore, considerable effort has recently been devoted to the development of an Avrami model for simultaneous reactions.⁷⁻¹⁴ Most of these works calculated the total volume of transformed product, but did not calculate the real volume of each transformed phase.

A simple method of accounting for two precipitates (1 and 2) is that the above equation becomes a set of

two equations

$$dV_1 = \left(1 - \frac{V_1 + V_2}{V}\right) dV_1^e \quad \dots \quad (3)$$

$$dV_2 = \left(1 - \frac{V_1 + V_2}{V}\right) dV_2^e \quad \dots \quad (4)$$

which in general must be solved numerically although an analytical solution which gives both V_1 and V_2 has been proposed for the case where the ratio of the volume fractions of the two phases is constant.¹¹ The method can in principle be extended to incorporate an indefinite number of reactions occurring together. The purpose of the present work is to generalise the previous work and to present analytical expressions for cases other than the constant ratio described above.

Method

To obtain the general relationship between real and extended volumes in simultaneous transformations, the variables are first redefined as follows

$$v_i = \frac{V_i}{V}, \quad v_i^e = \frac{V_i^e}{V}, \quad z = \sum_{j=1}^n v_j, \quad \text{and} \quad z^e = \sum_{j=1}^n v_j^e \quad (5)$$

where V_i ($i=1$ to n) is the real volume of the product phase i , and V_i^e is its extended volume.

From the same analysis as described above with the assumption of random microstructure development

$$dv_i = (1 - z) dv_i^e \quad \dots \quad (6)$$

Summing equation (6) from $i=1$ to n and using equation (5) gives

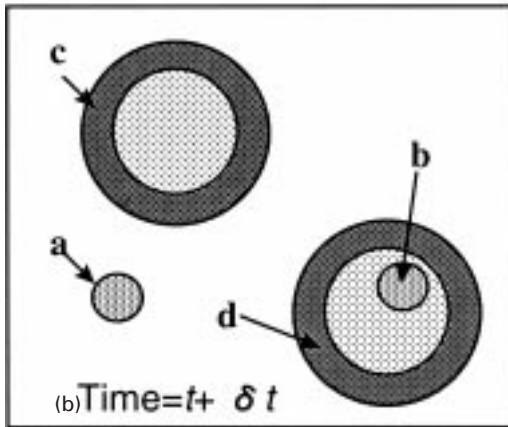
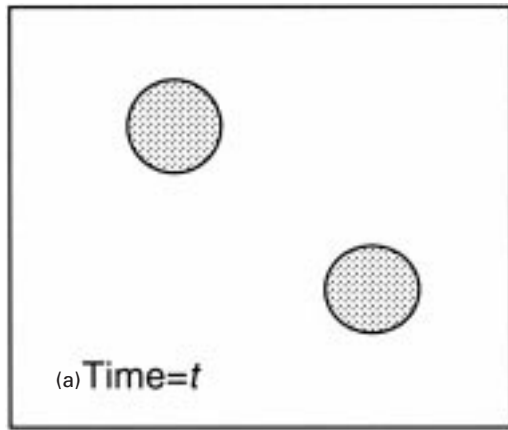
$$dz = (1 - z) dz^e \quad \text{and} \quad z = 1 - \exp(-z^e) \quad \dots \quad (7)$$

Equations (6) and (7) yield

$$dv_i = \frac{dv_i^e}{dz^e} dz = \frac{dv_i^e}{dz^e} (1 - z) dz^e = \frac{dv_i^e}{dz^e} \exp(-z^e) dz^e \quad \dots \quad (8)$$

Hence

$$v_i = \int \frac{dv_i^e}{dz^e} \exp(-z^e) dz^e \quad \dots \quad (9)$$



two precipitate particles have nucleated together and grown to finite size in time t ; new regions c and d are formed as original particles grow, but a and b are new particles, of which b has formed in region which is already transformed

1 Illustration of concept of extended volume

In equations (8) and (9), z^e is treated as the only independent variable, and v_i^e is considered to be a function of z^e . The calculations of v_i ($i = 1$ to n) require the relations between the various v_i^e values ($i = 1$ to n) throughout the reaction paths. To explain this necessary condition simply, two reaction paths, I and II, are considered, where the relations between the v_i^e values are different for the two paths. In this case, even if each v_i^e value is equal for reactions I and II at a certain moment, the v_i values are, at that moment, different because of the difference of the reaction paths. Determination of the relationships between the various v_i^e values throughout the reaction path is hence necessary to calculate v_i . Once all the v_i^e values are related to one another, only one v_i^e ($i = 1$ to n), or z^e , can be an independent variable. Equation (9) indicates that v_i can be calculated from only v_i^e ($i = 1$ to n) and gives the general relation between real and extended volumes.

Solution

Analytical solutions of equation (9) exist for special cases where the extended volumes of the different phases (or v_i^e for $i = 1$ to n) can be related. Hereafter, the case of $n = 2$ is considered and, for mathematical convenience, v_1^e is treated as an independent variable.

LINEAR

Suppose that v_1^e and v_2^e are related linearly according to

$$v_2^e = Bv_1^e - C \quad \dots \quad (10)$$

where B is a positive constant and C is zero or a positive constant. Since v_2^e cannot be negative, equation (10) implies that

$$z^e = \begin{cases} v_1^e & (0 \leq v_1^e \leq C/B) \\ (B+1)v_1^e - C & (v_1^e > C/B) \end{cases} \quad \dots \quad (11)$$

Equation (9) can then be integrated for $0 \leq v_1^e \leq C/B$ as

$$v_1 = 1 - \exp(-v_1^e) \quad \text{and} \quad v_2 = 0 \quad \dots \quad (12)$$

and for $v_1^e > C/B$ as

$$v_1 = 1 - \frac{B}{B+1} \exp(-C/B) - \frac{1}{B+1} \exp[-(B+1)v_1^e + C] \quad \dots \quad (13)$$

$$v_2 = \frac{B}{B+1} \{ \exp(-C/B) - \exp[-(B+1)v_1^e + C] \} \quad (14)$$

The new parameters $(v_1)_s$ and $(v_1^e)_s$ are defined here as v_1 and v_1^e respectively, obtained during the simultaneous transformation. The parameter $(v_1)_s$ is calculated by subtracting $[1 - \exp(-C/B)]$ from equation (13), hence

$$\begin{aligned} (v_1)_s &= \frac{1}{B+1} \{ \exp(-C/B) - \exp[-(B+1)v_1^e + C] \} \\ &= \frac{1}{B+1} \exp(-C/B) \{ 1 - \exp[-(B+1)(v_1^e - C/B)] \} \\ &= \frac{v_2}{B} \quad \dots \quad (15) \end{aligned}$$

The term $\exp(-C/B)$ occurs because $[1 - \exp(-C/B)]$ of phase 1 exists before commencement of the simultaneous reaction, and $(v_1^e - C/B)$ is $(v_1^e)_s$. Equation (15) shows that there is a simple linear relation between $(v_1)_s$ and v_2 . An example of an actual simultaneous reaction is a precipitation phenomenon in ferritic steel. Suppose that the isotropic growth rate of phase i ($i = 1, 2$) is G_i , and that all particles of phase i start growth at time $t = 0$ from a fixed number of sites N_i per unit volume, then

$$v_1^e = \frac{N_1}{V} \frac{4\pi}{3} G_1^3 t^3 \quad \text{and} \quad v_2^e = Bv_1^e \left(B = \frac{N_2 G_2^3}{N_1 G_1^3} \right) \quad (16)$$

It is emphasised that the specific assumptions made to express v_1^e can be selected at will, for example, to include a nucleation rate. Details can be found in Ref. 1. Equation (16) is the special case where C in equation (10) is zero, which has been used by Robson and Bhadeshia¹⁴ to examine the precipitation phenomena in power plant steel. A negative value of C would require a rearrangement of equation (10) with corresponding changes to the subsequent derivations.

PARABOLIC

The case is now discussed where v_1^e and v_2^e are related parabolically

$$v_2^e = A(v_1^e)^2 + Bv_1^e - C \quad (A > 0, \quad B, C \geq 0) \quad \dots \quad (17)$$

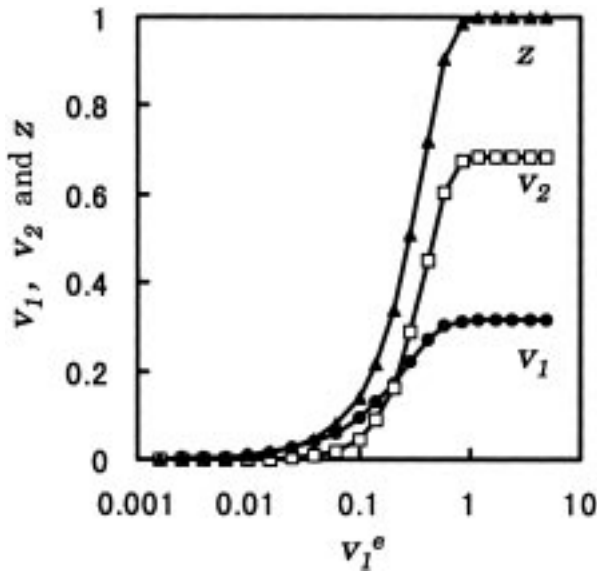
Equation (17) implies that when v_1^e is less than R ($\equiv [-B + (B^2 + 4AC)^{1/2}]/2A$), v_2^e is zero. Hence, for $v_1^e < R$, equation (9) becomes

$$v_1 = 1 - \exp(-v_1^e) \quad \text{and} \quad v_2 = 0 \quad \dots \quad (18)$$

and for $v_1^e \geq R$

$$v_1 = 1 - \exp(-R) + \exp\left[\frac{(B+1)^2}{4A} + C\right] \frac{1}{2} (\pi/A)^{1/2} \times [\text{erf}(\tau) - \text{erf}(\tau_0)] \quad \dots \quad (19)$$

$$v_2 = 1 - v_1 - \exp[-A(v_1^e)^2 - (B+1)v_1^e + C] \quad \dots \quad (20)$$



2 Calculation of v_1 and v_2 for case of parabolic relationship between v_1^e and v_2^e ($A=5$ and $B=C=0$ in equation (17))

Here, erf(τ) is the error function, and

$$\tau = A^{1/2} \left(v_1^e + \frac{B+1}{2A} \right) \quad \text{and} \quad \tau_0 = A^{1/2} \left(R + \frac{B+1}{2A} \right) \quad \dots \dots \dots (21)$$

v_i again indicates the phases that form simultaneously. Figure 2 shows the calculation results for $A=5.0$ and $B=C=0$.

So far, the present authors have found no example of parabolic relations for actual transformations. Since growth rate and number of nucleation sites (G_i and N_i in equation (16)) are not constant in general and B in equation (16) is thus not constant, the analytical solutions derived in the present work (equations (13), (14), (19), and (20)) do not always function conveniently for actual simultaneous

transformations. It is now, however, possible to examine simultaneous transformation phenomena systematically, because the general relation between v_i and v_i^e ($i=1$ to n), hence between real and extended volumes, has been given as equation (9).

Conclusion

The general relationship between real and extended volumes in simultaneous transformations has been considered, and analytical solutions derived for cases where extended volumes of two different phases are related linearly or parabolically. In practice, there are many instances where several transformations occur together, and the general relationship obtained in the present work renders it possible to examine their characteristics systematically.

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