

Mathematical Modelling Of Heat Treatment Processes

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Abstract- The aim of modelling of heat treatment processes is double, on the one hand, to know the details and connections of these with the material characteristics (mechanical, physical, etc.), on the other hand, to form the technologies being used in a factory. Both aims are not separated as the optimal technologies cannot be formed without knowledge of processes carrying out in the heat treatment. If the heat treatment consisted of only one process, the necessary time of heat treatment being given from the modelling (isotherm case) can easily be recalculated to the plant equipments. The base of the modelling is that the heat treatment regarded as a chain of thermal activated processes of Arrhenius-types can be written as one process having an (virtual) activation free enthalpy, thus, under certain conditions, the one-process model could already be used in non isotherm (industrial) cases too.

Keywords: heat treatment, process, mathematical model

I. INTRODUCTION

Heat treatments play very important rule in semi production, as on the one hand those are inevitable at the manufacture of product and, on the other hand, primarily determines their properties (mechanical, physical, etc.) being competent for the application. As the optimal technologies cannot be formed without the knowledge of processes carrying out during the heat treatment being understood by modelling at first. The base of the modelling is the interpretation of thermal activated process of Arrhenius-type and in present work that has investigated how to transform the description typically referring to the isotherm one-process into heat treatment consisting of multi- and, in each case, non isotherm processes [1].

II. MODELLING OF HEAT TREATMENT

A. Isotherm heat treatment

The rate of process(es) carrying out in the heat treatment can be written as follows

$$\frac{dx}{dt} = kX, \quad (1)$$

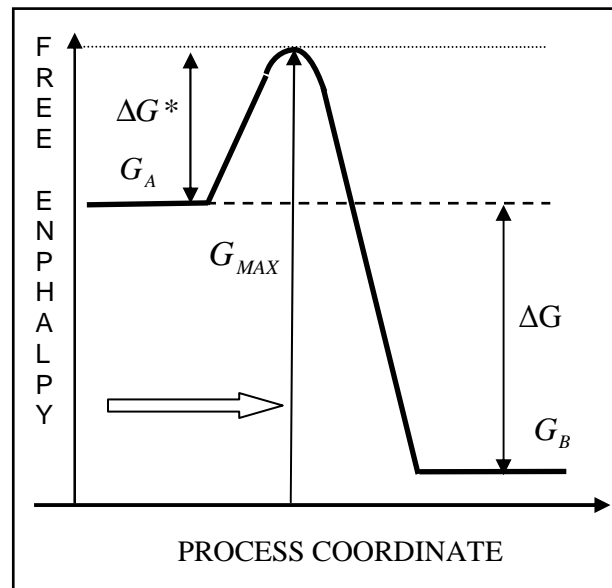


Figure 1. The interpretation of the activation free enthalpy

where $x(x=x(t))$ is the coordinate of process, meaning the ratio of that to the t time, k is the rate constant, which can usually be given as Arrhenius-type relation [2], namely

$$k = ae^{-\frac{\Delta G^*}{RT}}, \quad (2)$$

where ΔG^* is the so-called activation free enthalpy (Figure 1), T is the temperature of the process, R is the gas constant and x is the driving force, depending on the process coordinate, $X=X(x)$.

Integrating (1) from 0 to t the kinetics of the process can be calculated. Experimental investigation may be done by measuring some kind of material characteristics (electrical resistance, hardness, etc.) which is proportional to the process coordinate, that is

$$m = \beta x. \quad (3)$$

Rearranging (1) and writing (2) in that the latter can be formed as follows

$$\frac{dx}{X(x)} = ae^{-\frac{\Delta G^*}{RT}} dt. \quad (4)$$

Taking isotherm process ($T=\text{const}$, integrating (4) from 0 to x_p and from 0 to t_p , where t_p is the time belonging to x_p (p.e. $x_p=0.95$, because the time to the $x_p=1$ is usually infinite, $t = \infty$) can be given the next

$$t_p e^{\frac{\Delta G^*}{RT}} = \frac{1}{a} \int_0^{x_p} \frac{1}{X(x)} dx = A_p, \quad (5)$$

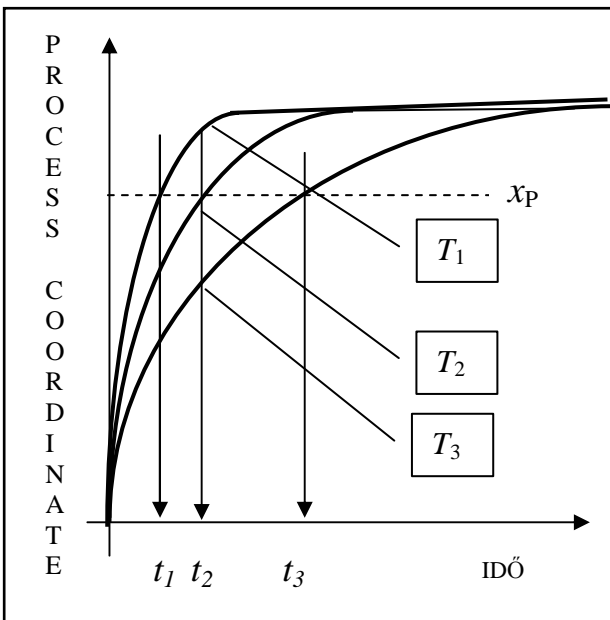
i.e. the product of temperatures and times of (5) needed to the taking place of process, x_p will be constant. The heat treatment time from (5) is

$$t_p = A_p e^{\frac{\Delta G^*}{RT}}. \quad (6)$$

The latter is usually expressed in logarithm form as it can be seen below

$$\ln t_p = \frac{\Delta G^*}{R} \frac{1}{T} + \ln A_p, \quad (7)$$

consequently, the heat treatment time as the function of reciprocal temperature will be straight lines, which slope is related to the activation free enthalpy (Appendix I.) and axial section, the pre-exponential coefficient is the function of thermodynamically driving force. Therefore it is successful to determine these two parameters, using of them the time of heat treatment belonging a chosen temperature can be calculated.



2. ábra. Determination of temperature-time pairs from the isotherm heat treatment curves.

The determination of parameters are down by the taking down of heat treatment curves at several temperatures (Figure 2) and the logarithms of times

belonging to x_p are plotted versus the function of reciprocal temperature $1/T$ (Figure 3)

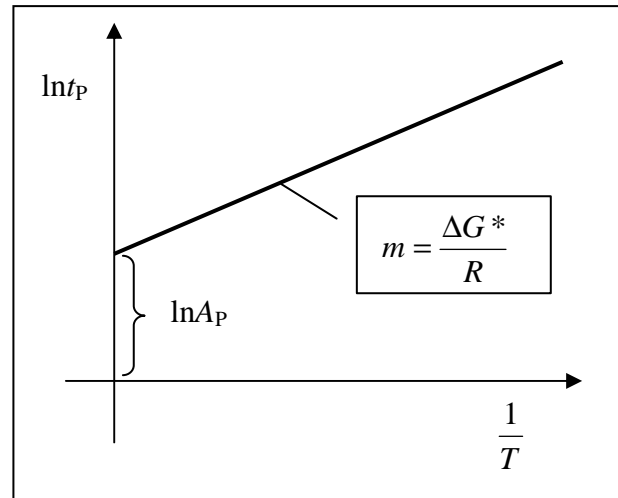


Figure 3. Determination of activation free enthalpy

Condition of adoption (7) is that neither the driving force, nor the activation free enthalpy (5) depends directly on the time only by way of process coordinate, x .

In case of one process or if there is one competent of processes carrying out during the heat treatment the activation free energy does not depend on the temperature of course, however, the driving force can depend on the temperature. For example, in case of precipitation process after quenching the driving force is related to the supersaturation of the solid solution and its measure decreases with the increase of temperature (the solubility increases) at the solvus temperature the driving force will be zero (C-curve) [3]. Therefore in this case those mentioned before may be used well over or under the solvus temperature, in a relatively narrow temperature interval.

B. Multi-processes model, effective activation free enthalpy

In case of parallel processes the time of heat treatment is determined by the time (activation free enthalpy) of competent process (p.e. in AlMg alloys the homogenization time is equal to the time of equalization of Mg, in AlMn alloys that will be the time of precipitation of Mn [4]). As these process are independent from one another (generally this can be supposed) the modelling mentioned before can be used as well.

In case of consecutive processes (n) using a linear process model, which means that the process $i+1$ starts by the time when the process i has been reached to a some extend ($x_0^{(i)}$), the time needed to carrying out of complete process will be

$$t_p = t_0^{(1)} + t_0^{(2)} + \dots + t_0^{(i)} + \dots + t_0^{(n-1)} + t_p^{(n)}, \quad (8)$$

where $t_0^{(i)}$ is the time of process i belonging to the start of process $i+1$. Using (5) the this latter will be the next

$$t_0^{(i)} = A_0^{(i)} e^{\frac{\Delta G_i^*}{RT}} \quad \text{and} \quad A_0^{(i)} = \frac{1}{a_i} \int_0^{x_0^{(i)}} \frac{1}{X(x_i)} dx_i \quad (9)$$

and $t_p^{(n)}$ is the process time of process n , namely

$$t_p^{(n)} = A_n e^{\frac{\Delta G_n^*}{RT}} \quad \text{and} \quad A_p^{(n)} = \frac{1}{a_n} \int_0^{x_p^{(n)}} \frac{1}{X(x_n)} dx_n. \quad (10)$$

There are two cases, one of them is when $x_0^{(i)} \rightarrow 0$, the processes closely follow each other, in this case the rate of total process is controlled by the slowest process (j). The activation free enthalpy of the total process will be

$$\Delta G^* = \Delta G_j^* \quad \text{and} \quad A_p^{(n)} = A_p^{(j)}, \quad (11)$$

the multi processes seem to be one process (quasi one process approximation) and (7) can be used in what follows too. For example at the precipitation along the grain boundary the slowest process is the diffusion of alloying elements to the grain boundaries, therefore the activation free enthalpy will be that of the diffusion process [3].

The other case is when $x_0^{(i)} \rightarrow 1$, the $i+1$ process $i+1$ starts by the time when the process i has been ended (chain process model). Then the time being necessary to playing of the total process as follows

$$t_p = t_p^{(1)} + t_p^{(2)} + \dots + t_p^{(i)} + \dots + t_p^{(n)}, \quad (12)$$

where the process times, $t_p^{(i)}$ as similar to (10) are

$$t_p^{(i)} = A_p^{(i)} e^{\frac{\Delta G_i^*}{RT}} \quad \text{and} \quad A_p^{(i)} = \frac{1}{a_i} \int_0^{x_p^{(i)}} \frac{1}{X(x_i)} dx_i. \quad (13)$$

Comparing (6), (12) and (13) an average activation free enthalpy can be defined, namely

$$\Delta \bar{G}^* = RT \ln \left(\sum_{i=1}^n \frac{A_p^{(i)}}{A_p} e^{\frac{\Delta G_i^*}{RT}} \right), \quad (14)$$

which is function of the temperature, T . Expand (14) into series to the first term that is

$$\Delta \bar{G}^* = \Delta G^*(0) + qT, \quad (15)$$

replacing (15) into a (6) the total process time will be

$$t_p = A_p e^{\frac{\Delta G^*}{RT}} = A_p e^{\frac{q}{RT}} e^{\frac{\Delta G^*(0)}{RT}} = A_p^* e^{\frac{\Delta G^*}{RT}}, \quad (16)$$

Arrhenius-type, where ΔG^* is an effective activation free enthalpy belonging to the total process, on the other word, in case of isotherm heat treatment the total (multi) process (n) can be regarded as one process with ΔG^* effective activation free enthalpy and A_p^* pre-exponential coefficient.

Within the total process different process (n -th) can be competent for the several characteristics. It means that the (effective) activation free enthalpies connecting to the several characteristics can be different from each other, therefore the pairs of temperature-time can be different as well. For example after the annealing of rolled products the yield stress is determined by disappearance of dislocations (decrease of dislocation density) while the elongation depends, beyond that, on the polygonization following that (size of polygons). Therefore different pairs of temperature-times of (7) will give the maximum values for the yield stress and elongation, however, there is a combination of those, when the characteristics mentioned before will be optimum [5].

III. MODELLING OF INDUSTRIAL HEAT TREATMENT

In case of heat treatment being carried out under industrial circumstances the times of heating up and cooling down need to be regarded (Figure 4). The total cycle time accordingly is

$$t_{CYCL} = t_{UP} + t_{HEAT} + t_{DOWN}. \quad (17)$$

The questions are the following : which will be the case when the results are equivalent with those given from isotherm heat treatment, if those are equivalent, how long is the heat time (the soaking time) t_{HEAT} as the only changeable parameter (the other two parameters can also be changed, but the change of those usually requires new apparatus (p.e. cooling or continuous heat treatment furnace, etc.).

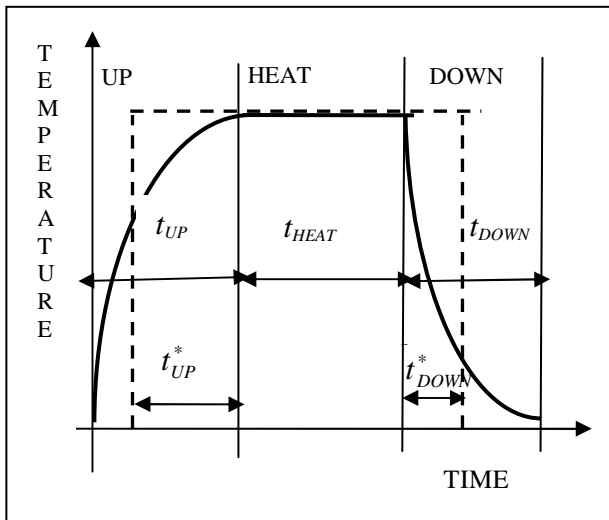


Figure 4. The diagram of temperature-time of an industrial heating furnace and substitution of that by times of model (isotherm)

One-process model

Be the temperature function of the time, than from (6) the equivalent times being convenient to the times of up heating- and down cooling will be

$$t_{UP}^* = \frac{A_0}{t_{UP}} \int_0^{t_{UP}} e^{\frac{\Delta G^*}{RT(t)}} dt, \quad (18)$$

$$t_{DOWN}^* = \frac{A_0}{t_{DOWN}} \int_{t_{CYCL} - t_{DOWN}}^{t_{CYCL}} e^{\frac{\Delta G^*}{RT(t)}} dt. \quad (19)$$

Both integrals can easily be calculated by the knowledge of temperature as function of times heat up and cooling. The soaking time

$$t_{HEAT} = t_0 - t_{UP}^* - t_{DOWN}^* \quad (20)$$

will be shorter and it would be at isotherm case (t_0).

B. Multi-processes model

In case of linear process model, if the processes closely follow each other, the total process can be regarded as one process (quasi one process approximation), therefore (18)-(21) can be used in what follows too.

In case of chain process the total process can be regarded as a quasi one process with (14) free enthalpy showing (15) dependence of temperature, which results an effective free enthalpy. At non-isotherm case an average free enthalpy can be defined as in (14), which depends on the time by means of temperature, $T(t)$. It means that the average free enthalpy depends on the heat up and cooling times, $\Delta \bar{G}^*(T, t_{UP}, t_{DOWN})$. Therefore the effective activation free enthalpy depends on the time too, thus calculation of (18)-(19) for the heat up and cooling times in the cycle time (17) cannot be used. In

this case the stages of heating up and cooling (non isotherm) need to be modelled, causing a lot of plus work [6]. Fortunately in this case there usually is a competent process, which is taken account an "incubation" process with incubation time of Arrhenius-type and that can be calculated in a relative simple way.

APPENDIX

I. Activation enthalpy

The free enthalpy consists of two parts, namely

$$G = H - TS \quad (A.1)$$

where H is the enthalpy and S is the entropy of process. In accordance with this the activation free enthalpy at isotherm process ($T=\text{const.}$) will be

$$\Delta G^* = \Delta H - T\Delta S \quad (A.2)$$

Writing (A.2) in (7) that is

$$\ln t_p = \frac{\Delta H^*}{R} \frac{1}{T} + \ln A_p - \frac{\Delta S^*}{R}. \quad (A.3)$$

The slope of the straight lines will be related to the ΔH^* , the activation enthalpy. The solid materials are incompressible, the enthalpy is equal to energy, therefore $\Delta H^* = E^*$, where E^* is the so-called activation energy. In biology the activation energy is generally used [7].

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