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Thermo-Mechanical-Metallurgical Model of Welded Steel†

Part I: Evolution Equations for Internal Material Structures

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Abstract

The transient and residual stress distribution in a welded joint is affected by solid-liquid and solid phase transformation in the HAZ. Metallurgical phenomena are coupled with stress and elastic strain in a dispersed material particle provided with a multiphase structure. Phase growth laws presented in the literature are given usually as exponential parabolic forms which are not suitable for incremental finite element analysis of a coupled thermo-mechanical-metallurgical problem of welding or quenching. Hence an attempt has been made to rectify the situation with transformation kinetic laws. A unified mathematical procedure applied to several transformation models yield phase growth laws in forms of evolution equations . Kinetic equations of various types have been reviewed to deduce the general forms of diffusional and diffusionless transformation laws. such generalised kinetic equations will be used in finite element formulation of welding problems with phase transformation

KEY WORDS: (Welding) (PhaseTransformation) (Microstructure of alloys) (Evolution Equations) (Kinetic equations) (Thermodynamics) (Gibbs energy)

1. Introduction

In simulation of welding, the model for heat flux generated by an arc or torch, the model for the welding bath, and the model of the heat affected zone (HAZ) are coupled. The weld pool and HAZ follow the arc or torch motion. In the weld pool two opposing processes: melting and solidification dominate. In the HAZ, a number of phenomena occur and the most important are: phase transformation, thermal dilatation, inelastic deformation, and transformation induced plasticity accompanying volumetric strain effects. Material state in thermo-mechanical-metallurgical process is defined by the following variables: the stress rate $\mathbf{S}$, the strain rate $\mathbf{E}$, temperature θ, and vector of phase fractions $\mathbf{y}$. The state variables called also constitutive variables are defined in a dispersed particle with internal multiphase structure, which is called the microregion. The dispersed particle is of the size of several grains and the Heat Affected Zone or its greater part is called the mesodomain. The microregion is considered here as a material portion like a particle in the classical continuum mechanics. State variables are coupled and coupling is provided by a system of three equations expressing: the balance of virtual work, the balance of internal energy, and evolution laws for phase fractions. The volumetric strain effects, transformation-induced plasticity, and plastic straining generate transient and residual stresses during welding and post-weld heat treatment. A reaction of welded material through thermo-mechanical-metallurgical process is determined by evolution laws for phase fractions, hardening parameters, constitutive equations for thermoelasticity, classical plasticity and transformation-induced plasticity. Forms of these equations show an influence of stress, strain, and temperature on the kinetics of phase transformation and, reversely, an effect of multi-phase material composition on material reaction under combined thermo-mechanical loading. In this thermo-mechanical-metallurgical modelling, it is required to know the temperature θ, density of each phase, thermal and mechanical properties, and their temperature dependent characteristics for every microregion at each time throughout the process.

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The main purpose of the first part of this paper is to give a summary of information related to thermodynamics and kinetics of phase transformation which is necessary to develop an algorithm for solution of thermo-mechanical- metallurgical problem of welding. Formulas for Gibbs free energy at nuclei, equations for the rate of nucleation, and numerical data related to micromechanics are presented together with evolution laws for phase transformation. This section of the paper is also an attempt to rectify the current situation with kinetic laws for diffusional and diffusionless phase transformations, and evaluate their applicability for simulation of HAZ during the cooling process. Basic postulates and notions for various transformation laws are studied and their final forms of ordinary differential equations, called evolution equations, are presented. These equations show relations between a phase fraction rate $\dot{y}_i$ and rates of quantities controlling a phase transformation expressed in terms of constitutive variables $\dot{\mathbf{S}}, \dot{\mathbf{E}}, \dot{\theta}$, and time t. Evolution equations are more suitable for incremental analysis and they can be used together with rate type balance laws derived for internal energy, and virtual work. Balance laws and evolution equations complete thermo-mechanical-metallurgical problem formulation. A brief study of mechanisms of phase transformation helps in motivation of basic assumptions for phase transformation modelling. Various types of phase growth laws are reviewed here and they are found to have heuristic or phenomenological nature. The kinetic laws are usually presented in the form of exponential parabolic equations which are not suitable for consistent incremetal thermo-plastic analysis. Hence evolution equations have been derived here for:

- the Johnson-Avrami-Mehl law [29], [41] for the partial pearlitic transformation which relates phase fractions of diffusional transformations with the rate of internal stress, temperature rate and time,
- the extended Koistinen-Marburger law [27], [28] for diffusionless transformation modified by internal stress and pressure, which relates the martensite fraction with the rate of hydrostatic pressure, the rate of equivalent stress, and temperature rate,
- the three-dimensional generalization of the kinetic law obtained from thermodynamics and statistical analysis, and shown in [39] for the uniaxial load. This relates the rate of martensitic fraction transformation with the rate of strain energy and the rate of temperature.

The evolution law originally proposed in [38] for the martensitic transformation and formulated following thermodynamical postulates is derived here from the basic assumption of proportionality of the martensitic fraction to an increment of the reaction driving force. This law relates the external loading stress and the average hydrostatic pressure with the rate of martensitic fraction, and can also be seen as a generalization of the Koistinen-Marburger parabolic equation.

Evolution laws reviewed here require more or less expensive identification of material parameters and functions due to the involvement of metallurgy in description of transformation kinetics. The comparison of different evolution laws accounting for metallurgical phenomena of various scales helps in choosing models which do not require expensive experiments for identification of material functions and model parameters.

Numerical schemes with FEM for several combinations of evolution laws for diffusional and diffusionless transformations, and derivations of the consistent or algorithmic tangent moduli for thermo-mechanical-metallurgical model of material and numerical results will be presented in the second part of this paper.

2. Phase Transformations

In making an attempt at modelling of phase changes, occuring due to welding of steel, the complexity of this task must be realized. Simultaneous processes which are coupled and accompanied with internal energy transformations make this task difficult. Simplifications in a mathematical description of welding process have been proposed after identification of physical mechanisms involved in complex thermo-mechanical-metallurgical phenomena The proposed model of the process compromises a target precision and non-complete physical treatment of material problems. A full physical treatment of such a problem may not be possible as the plastic deformation of a body and its thermal loading causes microstructure evolution, modification of volume fractions, chemical free energy changes, surface energy changes, and lattice deformation due to relief of internal stresses and formation of stress-free states [14]. Simplifications proposed for the mathematical description of solid phase transformations aim at representing coupled thermo-mechanical phenomena as a chain of successive processes, ignoring secondary reactions proceeding simultaneously which involve less internal energy than others, and idealizing the cooling process. An assumption of continuity of cooling is widely adopted as a common feature of phase transformation modelling.

2.1 Reactions and Transformations

Phase transformations in solids, like all chemical reactions, are caused by the free energy difference between a parent and a product phase. The difference is called a transformation driving force, and can be

aided by pressure, stress and strain as well as temperature. The majority of phase transformations, occurring in the solid state, take place by thermally activated atomic movement and they are called diffusional transformations. These transformations are induced by a change of temperature of an alloy of fixed bulk composition. The different types of transformations that are possible can be divided into the following five groups [10], [19], [41]:

- precipitation reaction,
- eutectoid transformation,
- ordering reaction,
- massive transformation,
- polymorphic changes.

The precipitation reaction transforms a metastable supersaturated solid solution, $Fe - C$-ferrite ie. α-phase into a more stable solid solution which is the low-carbon ferrite phase ie. α-phase and a stable precipitate ie. a high-carbon product cementite, Fe_3C. The eutectoid transformation consists of replacement of a metastable phase by a more stable mixture of two other phases. The pearlite reaction is the example of eutectoid transformation where the significant feature is the cooperative growth of two phases: the cementite, as well as the ferrite. The precipitation and eutectoid transformation are caused by a long-range diffusion which is involved when phases of different composition to the matrix are produced. The ordering reaction transforms the disordered phase into an ordered one. The massive transformation is characterized by short range diffusion and consists of a decomposition of the parent γ-phase into one or more daughter phases, which have the same composition as the original phase, but different crystal structures. A product of this transformation can either be stable or metastable. Such reactions can be illustrated by the remaining austenite transformation into martensite of a lath or bundle structure. The polymorphic transformation is observed in a single component system when different crystal structures are stable over different temperature ranges. This transformation can be illustrated by the transformation of the f.c.c.-Fe into the b.c.c.-Fe atomic arrangements. Ordering, massive, and polymorphic transformations proceed without any composition change and long-range diffusion.

In all metals and alloys the diffusional movement of atoms can be blocked by a rapid cooling, when a phase transformation can proceed by a cooperative movement of atoms which is an alternative mechanism of atomic movement. The diffusionless transformation which proceeds by cooperative movement of atoms during quenching is called the martensitic transformation. The product of this reaction is either bainitic ferrite, when reaction occurs below the Widmanstatten temperature, or martensite for transformation temperature below M_s. Martensite [36], [41] is characterized by: the atomic movement less than inter-atomic spacing, lack of chemical decomposition, the surface relief, and the presence of many lattice imperfections. The crystal structure of martensite obtained by quenching of austenite γ-phase in carbon steel has a body-centered tetragonal (b.c.t.) lattice which may be regarded as the α-lattice with one of cubic axes elongated. The tetragonality, measured by the relation of the elongated axis to the basal plane axis, and the volume of the unit cell increase with the carbon content.

Each transformation can be split into two stages: nucleation and growth. The nucleation can be seen as the new phase incubation period and will appear in analysis as time-delay of the growth period.

Emphasis has to be put on the fact that only two long-range diffusional reactions: precipitation and eutectoid transformation will be accounted for by kinetic laws postulated for diffusional transformations. The remaining three: ordering, massive, and polymorphic transformations will be neglected. These assumptions can be considered as the first step of phase change idealization. Further simplifications are related to a thermodynamical process occuring in a material portion.

2.1.1 Mechanisms of Diffusional Transformations

Three distinct steel phases are produced from the supersaturated γ-phase decomposition due to continuous cooling and two diffusional transformations: ferritic, and pearlitic. All quantities related to them will be marked by the subscript i. The subscript i assumes the following values: $i = 2$ for ferrite $i = 3$ for pearlite, and $i = 5$ for cementite. The allocation of values for i is arbitrary but the value $i = 1$ is reserved for austenite, $i = 4$ for bainite, and $i = 6$ for martensite, which is produced by the diffusionless reaction. Such arrangement of i values follows the transformation sequence.

The kinetic equations for diffusional phase transformations have been proposed for the idealized thermodynamical process based on the following assumptions [15], [20]:

- the body is subjected to the continuous cooling process,
- the microstructure obtained at the end of a continuous cooling is the result of a succession of elementary isothermal transformations, and each

one is independent of the preceding thermal history.

The later assumption is called **the additivity principle** and is the concept for approximation of a real cooling process which is different at each material point of the considered body $\mathcal{B}$. Hence the progress of an isothermal phase change can be conveniently represented by plotting the phase fraction $\mathbf{y}$ as a function of time t and temperature θ, i.e. the Transformation-Time-Temperature (TTT) diagram. The TTT diagram replaces the Continuous-Cooling-Transformation (CCT) diagram which must be given for each particular cooling process and material microregion. The phase fraction $\mathbf{y}(t, \theta)$ is determined by the following factors: the nucleation rate, the growth rate, the density and distribution of nucleation sites, overlapping of diffusion fields by adjacent transformed volumes, and the impingment of adjacent transformed volumes.
The metastable γ-phase (austenite) contains many nucleation sites after cooling and the following three schemes of transformation are possible:

- nucleation at the constant rate during the whole transformation,
- site saturation when all potential nucleation sites are consumed at the beginning of transformation,
- cellular transformation, when $\gamma \Rightarrow \alpha$ or $\gamma \Rightarrow \alpha + Fe_3C$.

The last scheme is most important for a description of transformations in steel because this reaction category contains the formation of pearlite and bainite, cellular precipitation, massive transformation and recrystallization. The cellular transformation can be terminated by the impingement of adjacent cells growing with the constant rate, that reveals an interaction between mechanical and metallurgical phenomena.

2.1.2 Mechanisms of Diffusional-Diffusionless Bainitic Transformation

The theory of bainitic reaction based on description of transformation mechanism has been developed in [2], [45], [46]. The bainitic reaction is partially diffusional and partially diffusionless transformation which has been indicated in [3], [4], [5], [6], [7]. The bainitic ferrite appears due to diffusionless-martensitic transformation after heterogeneous nucleation on the austenite grain boundary. Such ferrite sub-unit has a form of disc. "Sub-units" form a "sheaf" which grows by martensitic propagation of "sub-units". A "sheaf" size is limited by friction stress on "sub-units" boundaries. This stress oposes and finally terminates the growth of a sub-unit. The redistribution of carbon in ferritic sub-units occurs after actual transformation event due to carbide, Fe_3C, diffusional migration towards unit boundaries. The nucleation of bainitic ferrite is consistent with isothermal nucleation theory proposed in [6]. Hence, the activation energy for the bainitic reaction is a linear function of a chemical component of Gibbs free energy.

2.1.3 Mechanisms of Diffusionless Martensitic Transformation

The martensitic diffusionless transformation starts at the M_s temperature which depends on the carbon content in steel, and is also associated with a difference of Gibbs free energy between martensite and austenite. This difference is called the driving force and is influenced by internal pressure, external stress and temperature. The formation of martensite is a random process and this new phase appears in the shape of lens and spans. A martensitic plate in austenite grows in 10^{-5} to 10^{-7} seconds at velocity 800 to 1100 m/s and remains coherent with the austenitic matrix. The density of martensitic plates is not related to the grain size of austenite. The volume fraction of martensite increases by systematic transformation of the austenite remaining between the plates already formed. The martensitic transformation is terminated at the M_f temperature and further cooling does not increase the amount of martensite. The cooperative movement of atoms due to martensitic transformation is influenced by pressure, temperature and external stress. External tensile or compressive stress can increase the rate of martensitic nucleation when corresponding elastic strains contribute to the Bain strain produced by the Bain deformation due to the creation of the b.c.t. lattice from the f.c.c. atomic arrangement. In such cases the temperature M_s is raised [32], [40], [42] and the energy of such additional deformation provides the new term in the equation of the total free energy. The M_s is raised in a body under shear stress because the transformation driving force is reduced by a portion of the mechanical work performed by the shear stress [25], [26]. The M_s is affected only by stresses lower than yield stress [12] and it can not exceed the limiting value M_d even in appearance of plastic deformations. The temperature M_s can be suppressed to lower temperatures by hydrostatic compression [32] because of a stabilization of the close-packed austenite under high pressure. This effect decreases the atomic volume and reduces the transformation driving force ΔG_V.
Plastic deformation raises to some extent nucleation and growth of martensite but the large deformation can suppress the transformation. This mechanism can be explained by considering dislocations generated by plastic deformation and nucleation sites. The increase of dislocation density initially raises the number of

potential nucleation sites but large deformation may introduce restraints against the growth of nucleus.

2.2 Microstructure in Alloys

2.2.1 Microstructural Topology

The smallest piece of a multiphase polycrystalline alloy $\mathcal{B}$ of the size of one grain is called a **microregion** [17], [44] or dispersed particle. The microregion is composed of the manifold of particles such as eg. crystals. This microstructural element occupies a volume V_0^{mic} and has a surface A_0^{mic} at time $t = 0$. A much larger domain $\mathcal{M}$ which is an assembly of grains is called **mesodomain** and has a volume V_0^{mes} and a surface A_0^{mes}. The mesodomain contains a large number of microregions. A **phase** is a portion of the manifold of particles of an alloy whose properties and composition are homogenous and which is physically distinct from other properties of an alloy. The distribution of phases within a mesodomain is assumed statistically homogeneous. The mesodomain $\mathcal{M}$ and the microregion, at arbitrary time t, occupies the volume $V^{mes}(t)$ and $V^{mic}(t)$, respectively. Several nucleus sites can exist in one microregion and they generate a number of nuclei of the new phase. Each nucleus has its own volume V^{nuc} and a surface A^{nuc}.

2.2.2 Averaging over Mesodomain

An average value $\langle q \rangle$ over a mesodomain V^{mes} of arbitrary microscopic quantity $q(\mathbf{x})$, given in microregion V^{mic} is defined by the formula [17]

$$\langle q \rangle = \frac{\int_{V^{mes}} w(\mathbf{x}) q(\mathbf{x}) d\mathbf{x}}{\int_{V^{mes}} w(\mathbf{x}) d\mathbf{x}}, \tag{1}$$

where $\mathbf{x} \in V^{mes}$, and the weighting function $w(\mathbf{x})$ is the density distribution function [16] characterizing the crystallographic axes of the microregions. The example of such averaging is the evaluation of the macrofraction y^{mes} which measures the extent of transformation in the mesodomain V^{mes} and is defined by

$$y^{mes} = \frac{\int_{V^{mes}} w(\mathbf{x}) y^{mic} d\mathbf{x}}{\int_{V^{mes}} w(\mathbf{x}) d\mathbf{x}}, \tag{2}$$

where the microfraction y^{mic} is taken in the microdomain V_l^{mic}, and $\sum_{l=1}^{\mathcal{N}} V_l^{mic} = V^{mac}$. Latter the microfraction y^{mic} will be marked simply by y.

2.3 Free Energy and Nucleation

2.3.1 Gibbs Energy for Diffusional Transformations

Diffusional transformations: ferritic, and pearlitic are associated with heterogeneous nucleation. Hence, the change of Gibbs free energy driving such reactions is related to heterogeneous nucleation and has the following four contributions:

- a volume free energy reduction called also the chemical energy, $V_i^{nuc}\Delta G_{ch_i}$, caused by the creation of volume V_i^{nuc} of the new phase at temperature where this phase is stable,
- a free energy increase, $A_i^{nuc}\gamma_i$, caused by the creation of an area A_i^{nuc} of interface of the parent and daughter phase,
- strain energy, $V_i^{nuc}\Delta G_{\sigma_i}$, proportional to the volume of the new phase inclusion and given per unit volume,
- a free energy, ΔG_{d_i}, released by the destruction of a defect and reducing the activation energy barrier due to the creation of the new phase nucleus.

The subcsript i assumes here two values: $i = 2$ for ferritic transformation, and $i = 3$ for pearlitic reaction. The free energy change can be expressed as

$$\begin{aligned} \Delta G_i^{nuc} &= -V_i^{nuc}(\Delta G_{ch_i} - \Delta G_{\sigma_i}) \\ &+ A_i^{nuc}\gamma_i - \Delta G_{d_i}, \end{aligned} \tag{3}$$

where V_i^{nuc} is the nucleus volume, γ_i is the interfacial free energy per unit area and it is also the work that must be done at constant temperature θ to create unit area of phases interface. Units of ΔG_i^{nuc} are joules per nucleus. Ignoring the variation of γ_i with interface orientation and assuming the spherical shape of the new phase nucleus, Eq.(3) becomes

$$\begin{aligned} \Delta G_i^{nuc} &= -\frac{4}{3}\pi r^3(\Delta G_{ch_i} - \Delta G_{\sigma_i}) \\ &+ 4\pi r^2\gamma_i - \Delta G_{d_i}, \end{aligned} \tag{4}$$

where r is a diameter of the spherical nucleus. The critical value of r can be evaluated by differentiation of the RHS with respect to r, and comparing $\frac{\partial \Delta G_i^{nuc}}{\partial r}$ to zero. These operations yield

$$\begin{aligned} r^* &= \frac{2\gamma_i}{\Delta G_{ch_i} - \Delta G_{\sigma_i}}; \\ \Delta G_i^* &= \frac{16\pi\gamma_i^3}{3(\Delta G_{ch_i} - \Delta G_{\sigma_i})^2}, \end{aligned} \tag{5}$$

where ΔG_i^* is the critical value of the free energy ΔG_i^{nuc}.
The rate of heterogeneous nucleation [41] is given by

$$N_i = \omega_i C_{1_i} \exp\left(-\frac{\Delta G_{m_i}}{k_B\theta}\right) \exp\left(-\frac{\Delta G_i^*}{k_B\theta}\right), \tag{6}$$

where ω_i is the factor that includes the vibration frequency and the area of the critical nucleus, C_{1_i} is the concentration of heterogeneous nucleation sites per unit volume, ΔG_{m_i} is the activation energy for atomic migration per atom, ΔG_i^* is a change of Gibbs free energy for the critical nucleus diameter r_i^*, k_B is the

Boltzman constant. The Bolzman constant is given by $k_B = R/N_a$, where N_a is the Avogadro number equal to $6.023 \times 10^{+23}$ and R is the universal gas constant. The rate of nucleation gives number of nuclei per cubic meter and per second, and the unit of N_i is [nuclei $m^{-3}s^{-1}$].

2.3.2 Gibbs Energy for Diffusionless Transformations

Two phases are produced due to diffusionless transformations: bainitic ferrite, and martensite. Bainitic ferrite is marked with subscript $k = 4$, and quantities related to martensite are labelled by subscript $k = 6$.

The Gibbs free energy associated with the formation of one coherent inclusion, which appears due to diffusionless transformation, see [41], [30], is expressed as:

$$\Delta G_k^{nuc} = A_k^{nuc}\gamma_k + V_k^{nuc}(\Delta G_{\sigma_k} - \Delta G_{ch_k}), \qquad (7)$$

where $A_k^{nuc}\gamma_k$ is the elastic coherency interfacial energy, γ_k is the austenite-daughter phase interfacial free energy, ΔG_{σ_k} is the strain energy, ΔG_{ch_k} is the volume free energy release, V_k^{nuc} is the nucleus volume, and A_k^{nuc} is the nucleus surface. The strain energy of the coherent nucleus is more important than the surface energy because of high shear strain producing relatively large strains in the austenitic matrix. Moreover, twinning of a nucleus is also evaluated by shear strain.
A martensitic or bainitic ferrite nucleus is considered as a thin ellipsoidal disc, with radius a and thickness $2c$.
The free energy Eq.(7) for the coherent nucleus generated by a simple shear strain, s, can be written

$$\Delta G_k^{nuc} = 2\pi a^2\gamma_k + \frac{4}{3}\pi(s^2\mu a c^2 - a^2 c\,\Delta G_{ch_k}), \qquad (8)$$

where γ_k is the coherent interfacial energy, μ is the elastic shear modulus of austenite. The critical nucleus dimensions a^* and c^* can be found differentiating Eq.(8) with respect to a and c, and comparing derivatives: $\frac{\partial \Delta G_k^{nuc}}{\partial a}$, and $\frac{\partial \Delta G_k^{nuc}}{\partial c}$ to zero. The critical dimensions are expressed by

$$\begin{aligned} c^* &= 2\gamma_k \,/\, \Delta G_{ch_k}; \\ a^* &= 4\gamma_k\mu s^2 \,/\, (\Delta G_{ch_k})^2. \end{aligned} \qquad (9)$$

Substituting the above results into Eq.(8) yields an expression for the maximum value of ΔG_k^{nuc}

$$\Delta G_k^* = \frac{32}{3}\frac{\gamma_k^3}{{\Delta G_{ch_k}}^4} s^4\mu^2\pi. \qquad (10)$$

The nucleation barrier to form coherent nuclei can be reduced by the elastic strain field of dislocation which interacts with the strain field of the martensite nucleus and results in the reduction of the total energy of nucleation. Such interaction modifies the total free energy Eq.(7) which can be written [49] by

$$\begin{aligned} \Delta G_k^{nuc} &= A_k^{nuc}\gamma_k - \Delta G_d \\ &+ V_k^{nuc}(\Delta G_{\sigma_k} - \Delta G_{ch_k}), \end{aligned} \qquad (11)$$

where ΔG_d is the energy of dislocation interaction which reduces the nucleation energy barrier. Assuming that a complete loop of dislocation is interacting with the nucleus, the interaction energy is expressed by

$$\Delta G_d = 2\pi a c\,\mu\, s\, b, \qquad (12)$$

where b represents a length of the Burgers vector of dislocation. Subtracting Eq.(12) from the RHS of Eq.(8) results in the expression of the total energy of a martensite nucleus

$$\begin{aligned} \Delta G_k^{nuc} &= 2\pi a^2\gamma_k + \frac{4}{3}\pi(a c^2\mu\, s^2 \\ &- a^2 c\,\Delta G_{ch_k}) - 2\pi a c\,\mu\, s\, b. \end{aligned} \qquad (13)$$

The energy ΔG_k^{nuc} is related to diameter a and thickness c of the ellipsoidal disc representing a nucleus, the simple shear strain s, and the strain field generated by dislocation.

3. Kinetics of Transformation

The unified mathematical approach has been applied to all reviewed kinetic laws which can be derived from a basic assumption of proportionality of the new phase increment and a variation of a model variable which is controlling a transformation. The following quantities: time, temperature, stress, a reaction driving force, and a potency of material structural defects are considered here as variables controlling phase changes. The growth laws for phase fraction are expressed usually in the form of parabolic laws or ordinary differential equations called also evolution equations. Evolution laws reveal a rate type nature of interactions between constitutive variables and a transformation products.

3.1 Kinetics of Diffusional Transformations

3.1.1 Kinetic Equations for Ferritic and Pearlitic Transformations

The kinetic equation for two diffusional transformations: ferritic, and pearlitic, has the form of the parabolic growth law known as the Johnson-Avrami-Mehl equation [29], [41]

$$y_i = 1 - \exp(-b_i\ t^{n_i}), \qquad (14)$$

where y_i is the volume fraction of i-th phase in the considered microregion V^{mic}, n_i and b_i are empirical

parameters related to cooling rate and the nucleation rate, t is time equal to zero at the end of the nucleation period. This equation can be derived from the basic assumption that the daughter phase increment dy_i is proportional to the decrement of transformation driving force measured by the differential of the Gibbs free energy, $d\Delta G_i^{mic}$ where $i = 2$ or 3 for ferritic and pearlitic reactions. Therefore, the Johnson-Avrami-Mehl equation can be expressed in one of the following incremental forms:

$$\frac{dy_i}{d\mathcal{G}} = 1 - y_i; \tag{15}$$

$$\frac{dy_i}{1 - y_i} = d\mathcal{G}; \tag{16}$$

$$\frac{\dot{y}_i}{1 - y_i} = \dot{\mathcal{G}}, \tag{17}$$

where the differential of the Gibbs free energy is denoted by

$$d\mathcal{G} = d\Delta G_i^{mic}. \tag{18}$$

Identifying the rate of the Gibbs free energy change, $\dot{\mathcal{G}}$, as an explicit function of time

$$\dot{\mathcal{G}} = n_i\ b_i\ t^{n_i - 1}, \tag{19}$$

and substituting to Eq.(17) yields to the expression

$$\frac{dy_i}{1 - y_i} = n_i\ b_i\ t^{n_i - 1}\ dt. \tag{20}$$

The following operations gives the parabolic growth law Eq.(14) for ferritic and pearlitic transformations:

- Integration of Eq.(20) gives

$$\ln(1 - y_i) = -b_i\ t^{n_i}. \tag{21}$$

- Expressing the above in exponential form leads to

$$1 - y_i = \exp(-b_i\ t^{n_i}). \tag{22}$$

Eq.(14) was originally proposed for the case when the cells of the new phase were continuously nucleated throught the transformation at a constant rate. Example values of parameters n_3 and b_3 are given in [21] for for austenite-pearlite transformation for 1080 steel. The exponent n_i is not related directly to temperature as long as the nucleation mechanism does not change during cooling. The growth parameter b_i is temperature dependent [41] and related to both the rate of heterogeneous nucleation $N_i(\theta)$, see Eq.(6), and the cell growth rate $\nu_i(\theta)$. This is defined by

$$b_i(\theta) = \frac{1}{3}\pi N_i(\theta){\nu_i}^3(\theta). \tag{23}$$

The phase growth law expressed by Eq.(14) assumes the complete transformation of austenite into the new phase. Such reaction does not proceed instantaneously and therefore the growth law appropriate for the partial transformation during a continuous cooling process is defined by introducing the fictitious fraction [20], [22]

$$y_i^{\phi} \equiv \frac{y_i}{y_\gamma\ y_{i_{max}}} = 1 - \exp[-b_i(\theta)\ t^{n_i}], \tag{24}$$

where $y_{i_{max}}$ is the final fraction of phase i, and y_γ is the fraction of austenite at the beginning of transformation i.
Expressing Eq.(24) in the logarithmic form

$$\ln(1 - y_i^{\phi}) = -b_i(\theta)\ t^{n_i}, \tag{25}$$

and differentiating this with respect to time t, yields the following evolution equation

$$\frac{\dot{y}_i^{\phi}}{1 - y_i^{\phi}} = t^{n_i}\left[\frac{db_i}{d\theta}\ \dot{\theta} + \frac{b_i(\theta)n_i}{t}\right]. \tag{26}$$

3.1.2 Modified Kinetics

The kinetics of isothermal decomposition of austenite is influenced by hydrostatic pressure and stress [1], [12], [15]. The effect of hydrostatic pressure is observed as a decrease of the temperature A_3 of $\gamma - \beta$ iron transformation, a reduction of the eutectoid temperature A_1 of the $Fe - C$ diagram, and shifting the eutectoid transformation point toward lower carbon composition [18], [24], [35]. Following these modifications of specific temperatures and the eutectoid point relocation, the TTT and CCT diagrams show a displacement of curves towards longer transformation times and lower temperatures. Tensile or compressive stresses have the opposite effect on the pearlitic transformation as they accelerate the transformation and result in displacing of the TTT and CCT curves towards shorter times of transformation [37].

The nucleation and growth rates are influenced by the stress [13], [37], and such effect is modelled by relating material parameter b_3 of the Johnson-Avrami-Mehl model with the nucleation rate N_3. The situation with the exponent n_3 is vague because it is either decreasing [37] or increasing [13] respectively to internal stresses.

The influence of internal stress on kinetics of the pearlitic transformation has been presented in [13]. This concept consists of shifting of TTT diagrams either towards shorter times for tensile and compressive stresses or towards longer times for hydrostatic pressure. The shift D of the TTT diagram is postulated as the function of the second invariant J_2' of the Piola Kirchhoff stress deviator $\mathbf{S}$, the spherical part

of stress ie. hydrostatic pressure, and the second invariant I_E of plastic Green-Lagrange strain $\mathbf{E}^{pl}$. This relation can be written as

$$D = \mathcal{F}_D(J_2', p, I_E), \tag{27}$$

where $J_2' = [\frac{1}{2}\mathbf{S}{:}\mathbf{S}]^{\frac{1}{2}}$, $I_E = [\frac{2}{3}\mathbf{E}^{pl}{:}\mathbf{E}^{pl}]^{\frac{1}{2}}$, $p = \frac{1}{3}\, S_{KK}$, and ":" means the full contraction of the second order tensor.
The simple example of $\mathcal{F}_D$, shown in [13], is given by the linear function of J_2', such that,

$$D = C\, J_2', \tag{28}$$

where $C = 8.5 \times 10^{-3}\ \ [MPa]^{-1}$ for the isothermal transformation at temperature $\theta = 663°C$.

Postulating relation between the growth parameter b_i and the shift D in the form

$$b_{D_i} = \frac{b_i}{(1-D)^{n_i}}, \tag{29}$$

and substituting this to Eq.(24), the modified growth law for the partial transformation becomes

$$y_i^{\phi} \equiv \frac{y_i}{y_\gamma\ y_{i_{max}}} = 1 - \exp(-b_{D_i}\ t^{n_i}). \tag{30}$$

A plastic deformation of austenite grains during the pearlitic transformation, called the transformation induced plasticity, TRIP, acts almost similarly as tensile and compressive stresses, and results in shifting of the TTT and CCT curves towards shorter times. The TRIP effect accelerates the phase transformation [12], [33], [37], [48], [52] by increasing the rate of hetereogeneous nucleation N_i .
The evolution equation for Eq.(30) with Eq.(29) and Eq.(28) can be expressed in the following form

$$\frac{\dot{y}_i^{\phi}}{1-y_i^{\phi}} = \frac{t^{n_i}}{(1-CJ_2')^{n_i}}\left[\frac{db_i}{d\theta}\dot{\theta} + \frac{b_i(\theta)n_i C}{1-CJ_2'}\,\frac{dJ_2'}{d\mathbf{S}}\,\dot{\mathbf{S}} + \frac{b_i(\theta)n_i}{t}\right], \tag{31}$$

where the relation between rates of the phase fraction, temperature and stress is written explicitly.

3.2 Kinetics of Diffusional-Diffusionless Bainitic Transformation

The kinetic equation for the bainitic transformation proposed in [2], [45] is based on the assumption of the linear relation between an increment of the bainitic volume fraction dy_4^{ϕ} and volume increment of nucleus dN_4. This can be written as

$$\gamma\, dy_4^{\phi} = \left(1 - y_4^{\phi}\right) V^{mic}\langle dN_4\rangle; \qquad \gamma = y_\gamma y_{4_{max}}\ \ ; y_4^{\phi} = \frac{y_4}{\gamma}, \tag{32}$$

where $y_{4_{max}}$ is the maximum volume fraction of bainite, y_γ is the fraction of residual austenite, V^{mic} is the volume of a microregion, $\dot{N}_4 = \frac{dN_4}{dt}$ is the nucleation rate per unit volume, and angular brackets $\langle\rangle$ mean the volume average. Division of both sides of Eq.(32) by time increment dt leads to the rate type form of the bainitic transformation kinetic law

$$\frac{\dot{y}_4^{\phi}}{1-y_4^{\phi}} = \frac{V^{mic}}{\gamma}\langle\dot{N}_4\rangle \tag{33}$$

Nucleation of bainite sub-unit starts below the Widmanstatten temperature W_s. The nucleation rate $\dot{N}_4$ is related to quantities measured on two graphs: the first is a free energy diagram, which consists of free energy curves for ferrite and austenite versus a carbon content, and the second is the universal curve representing the minimum free energy change, which is necessary for displacive nucleation of ferrite at temperature W_s. The G_N is the value measured on the universal curve of minimum energy. The change of maximum nucleation free energy, $\Delta G_{4_{max}}$, is determined from the free energy diagram following a procedure described in [8], [23]. This method consists of the estimation of the free energy change as a distance between two parallel straight lines which are tangents respectively to ferrite and austenite energy curves. Knowing the content of carbon at a nucleus, a locus on the austenite free energy curve, and the corresponding tangent direction can be found. When such direction is known, the parallel line, which is tangent to the second curve, can be drawn. The location of a common point of a curve and a tangent line determines a carbon content at the bainitic ferrite.

The magnitude of $\Delta G_{4_{max}}$ exceeds value G_N at temperature W_s. The nucleation rate is expressed in terms of $\Delta G_{4_{max}}$, its initial value $\Delta G^0_{4_{max}}$, and value G_N. This can be written in the form

$$\Delta G_{4_{max}} = \Delta G^0_{4_{max}} - y_4^{\phi}\left(\Delta G^0_{4_{max}} - G_N\right). \tag{34}$$

The nucleation rate of bainite is defined in [45] by the following expression:

$$\langle\dot{N}_4\rangle = K_1 \exp\left(-\frac{K_2}{R\,\theta} - \frac{K_2\langle\Delta G_{4_{max}}\rangle}{r\,R\,\theta}\right), \tag{35}$$

where K_1 is the parameter related to austenite grain size, K_2 is constant, R is the gas constant, and r is the positive constant which appears in approximation of G_N given by

$$G_N = p\ W_s - r, \tag{36}$$

with $p = 3.6375$, and $r = 2540\ [J\ mol^{-1}]$. The parameter K_1 is a linear function of austenite grain size as has been postulated in [45].

Substituting Eqs.(34),(35) to Eq.(33), the evolution equation for bainitic transformation can be expressed by

$$\frac{\dot{y}_4^\phi}{1-y_4^\phi} = \frac{V^{mic}K_1}{\gamma}\left(1-\beta\,\gamma y_4^\phi\right)\times$$
$$\exp\left[\langle\Gamma_2\rangle y_4^\phi - \frac{K_2}{R\,\theta}\left(1-\frac{\langle\Delta G^0_{4_{max}}\rangle}{r}\right)\right]; \qquad (37)$$
$$\langle\Gamma_2\rangle = \frac{K_2\langle\Delta G^0_{4_{max}} - G_N\rangle}{r\,R\,\theta},$$

where β is the autocatalysis factor. The effect of autocatalysis is observed when the increase of the ferrite volume fraction is accompanied with the increase in number density of nucleation sites.

An analytical solution of Eq.(37), shown in [45], is obtained for the time t taken to form bainitic volume fraction y_4^ϕ at reaction temperature θ. This can be written as

$$t = \frac{\gamma}{M(\mathcal{G}^0,\frac{1}{\theta})}\left[-A\ln(1-y_4^\phi)+\right.$$
$$\left.\frac{B}{\gamma\beta}\ln(1-\beta\gamma y_4^\phi)+\frac{C}{\langle\Gamma_2\rangle}\left(1-\mathrm{e}^{-\langle\Gamma_2\rangle y_4^\phi}\right)\right]; \qquad (38)$$
$$M(\mathcal{G}^0,\frac{1}{\theta}) = V^{mic}K_1\exp\left(-\frac{K_2}{R\,\theta}-\frac{K_2\langle\mathcal{G}^0\rangle}{r\,R\,\theta}\right);$$
$$\mathcal{G}^0 = \Delta G^0_{4_{max}},$$

with parameters $A.B,C$ defined in [2] as following:

$$A = \frac{\exp(-\Gamma)}{1+\beta\,\gamma};$$
$$C = \frac{1-\exp\left(\frac{\Gamma}{\beta}\right)\left[1-\frac{1}{\beta}+\frac{A}{\beta}+A\gamma\right]}{\left[1+\gamma-\exp\left(\frac{\Gamma}{\beta}\right)\right]\left(1-\frac{1}{\beta}\right)}; \qquad (39)$$
$$B = 1-A-C,$$

where the factor

$$\Gamma = 11\,\frac{\mathcal{G}^0}{R\,\theta}, \qquad (40)$$

is related to reduction of the driving force for nucleation as y_4^ϕ increases.

3.3 Kinetics of Diffusionless - Martensitic Transformation

Kinetic equations for martensitic transformation can be divided into three groups:

- heuristic laws,
- relations derived from thermodynamics and statistics,
- equations derived form thermodynamics of continua.

3.3.1 Heuristic Laws

Heuristic laws are represented by the Koistinen-Marburger law [31] and its modifications proposed in [27], [28] and [51] which were obtained from identification techniques to achieve the best coincidence of a transformation model with experiment. The Koistinen-Marburger law is based on the assumption of the linear relation between the martensitic fraction increase $d\hat{y}_6$ and temperature decrease $d\theta$ below the temperature M_s where martensitic transformation starts. This can be expressed by

$$\frac{d\hat{y}_6}{d\theta} = \alpha\,(1-\hat{y}_6); \qquad (41)$$
$$\hat{y}_6 = \frac{y_6}{1-y_{2\div5}},$$

with the constant coefficient α which for most steels equals to $1.1\times10^{-2}[K^{-1}]$, and $y_{2\div5} = \sum_{i=2}^{5} y_i$ accounted for fractions of already formed phases.

Taking all terms of Eq.(41) with $\hat{y}_6$ to the left

$$\frac{d\hat{y}_6}{1-\hat{y}_6} = \alpha\,d\theta, \qquad (42)$$

introducing the new variable $z = 1-\hat{y}_6$, and integrating

$$\int_1^z \frac{1}{\xi}d\xi = \alpha\int_{M_s}^{\theta} d\vartheta, \qquad (43)$$

the Koistinen-Marburger law can be written in the form

$$\ln\xi\,|_1^z = \alpha(\theta - M_s), \qquad (44)$$

which is equivalent to

$$\ln(1-\hat{y}_6) = -\alpha(M_s-\theta). \qquad (45)$$

This relation reveals the exponential form of kinetic equation for martensitic transformation, i.e.

$$\hat{y}_6 = 1-\exp[-\alpha(M_s-\theta)]. \qquad (46)$$

The simple evolution equation for the martensitic fraction can be obtained from Eq.(42) assuming α constant, and $\hat{y}_6(t)$, $\theta(t)$ being functions of time

$$\frac{1}{1-\hat{y}_6}\dot{\hat{y}}_6 = \alpha\dot{\theta} \qquad (47)$$

with the initial condition $\hat{y}_6(0) = 0$ for $\theta(0) = M_s$. However, parameter α depends on: composition of the alloy, crystallography of the martensite habit planes, cooling rate, stress state, and is somehow related to transformation driving force ΔG_6^{mic}.

The improved Koistinen-Marburger law which accounts for the effect of pressure and stress on transformation temperature has been proposed in [27], [28]. The modification of M_s is a linear function of hydrostatic pressure and the equivalent stress

$$\Delta M_s = A\,p \;+\; B\,\hat{S}, \tag{48}$$

where A and B are material parameters, and $\hat{S} = (J_2')^{\frac{1}{2}}$.
Substituting Eq.(48) in Eq.(46) results in the extended Koistinen-Marburger law

$$\hat{y}_6 = 1 - \exp[-\alpha(M_s - \theta + Ap + B\hat{S})]. \tag{49}$$

Differentiation of the logarithmic form of Eq.(49) in respect of time yields the evolution equation corresponding to the extended Koistinen- Marburger law

$$\frac{1}{1-\hat{y}_6}\dot{\hat{y}}_6 = \alpha(A\dot{p} + B\frac{\partial \hat{\mathbf{S}}}{\partial \mathbf{S}}\dot{\mathbf{S}} - \dot{\theta}) \tag{50}$$

with the initial condition $\hat{y}_6(0) = 0$ for $\theta(0) = M_s$, $p(0) = 0$, and $\hat{S}(0) = 0$.
The other proposition of the modified Koistinen-Marburger law is given in [17], [51] and has the form

$$\begin{aligned} \hat{y}_6 &= \{1 - \exp[-\alpha_G(M_s - \theta) - \mathcal{E} : \mathcal{S}]\}; \qquad (51)\\ \alpha_G &= k_M V^{mic}\langle\frac{\partial \Delta G_6^{mic}}{\partial \theta}\rangle;\ \ \mathcal{E} = k_M V^{mic}\mathbf{E}_c^*, \end{aligned}$$

where $\mathcal{S}$ is the global stress tensor corresponding to the macroscopic strain tensor $\mathbf{E}$, ΔG_6^{mic} is the difference of the free energy per unit volume of the microregion, parentheses $\langle\cdot\rangle$ mean the average of $\frac{\partial \Delta G_6^{mic}}{\partial \theta}$ over the mesodomain, $\mathbf{E}_c^*$ is the critical value of the macroscopic strain reached when entire microregion transforms to martensite i.e. $y_6 = 1$, V^{mic} is the microregion volume, anad k_M is a proportionality factor defined by Magee [34], such that

$$k_M = \frac{dn}{dG}\ ; dG = \langle d\Delta G_6^{mic}\rangle, \tag{52}$$

with the number n of microregions transforming to martensite per unit volume of parent phase.
The evolution equation for Eq.(52) is not presented here because of detailed study of more advanced thermodynamical model encompassing effects of stress, strain and driving force on a phase transformation, which is given in the following subsection.

3.3.2 Kinetic Equation Arising from Thermodynamics and Statistics

A growth law proposed in [39] is the example of the kinetic equation obtained from thermodynamics and statistical analysis. This kinetic law for martensitic transformation is based on the identification of the fraction $\hat{y}_6$ with the probability ρ_{prob} and written in the form

$$\hat{y}_6 \equiv \rho_{prob} = 1 - \exp[-V^{mic}N_V(n)], \tag{53}$$

where ρ_{prob} measures the probability [11] that at least one nucleation site is contained in V^{mic}, and $N_V(n)$ is a cumulative structural defect potency defined by

$$N_V(n) = N_V^0\ \exp(-\alpha\, n) \tag{54}$$

with the total number density of defects of all potencies N_V^0, a constant shape factor α, and the defect size parameter n. The parameter n is postulated in the form

$$n = \frac{2\,\gamma_6}{\Delta G_6^{mic}\,d_6}; \tag{55}$$

with the close-packed interplanar spacing d_6, the nucleus specific interfacial energy γ_6, and the total volume free-energy change ΔG_6^{mic}. The free-energy change in diffusionless transformation, previously given by Eq.(7), is expressed now by

$$\Delta G_6^{mic} = A_6^{mic}\gamma_6 - \Delta G_{ch_6}^{mic} + \Delta G_\sigma^{mic} + \Delta G_F^{mic}, \tag{56}$$

where ΔG_σ^{mic} is the strain energy generated by internal stress and strain, and ΔG_F^{mic} is the frictional work of interfacial motion. The cumulative structural defect potency N_V is modified by the change of mechanical energy on habit planes, and is given

$$\begin{aligned} N_V(\mathcal{G}_\sigma) &= \int_{\mathcal{G}_\sigma}^{\mathcal{G}_\sigma^{max}} M(\mathcal{G})\exp[-\alpha n(\mathcal{G})]d\mathcal{G}; \qquad (57)\\ \mathcal{G}_\sigma &= \Delta G_\sigma^{mic};\\ \mathcal{G}_\sigma^{max} &= \Delta G_\sigma^{max}, \end{aligned}$$

where $M(\mathcal{G})$ is a linear function of $\frac{dN_V^0(\mathcal{G})}{d\mathcal{G}}$, and ΔG_σ^{max} is the maximal change of mechanical energy on habit planes which will be defined later.

The mechanical contribution of ΔG_6^{mic} is orientation dependent and requires a decomposition of the true stress vector in microregion $\vec{\mathbf{t}}$ into its normal $\vec{\sigma}^h$ and tangential $\vec{\tau}^h$ components on each habit plane h. The true stress is assumed to be homogeneous in a microregion V^{mic}. The total number of habit planes H is a sum of habit planes of b.c.c. austenitic crystals in a microregion. Each habit plane has the same area A^{hab}. The true stress vector respectively to the Kirchhoff (or Treftz) stress tensor t_{ij} is defined by

$$t_i^h = \frac{\rho}{\rho_0}t_{ij}n_j^h \tag{58}$$

with initial and actual density ρ_0 and ρ, and directional vectors $\mathbf{n}^h$ which define the orientation of the

h-th habit plane normal. Components of such vectors are given by

$$n_i^h = cos2\vartheta_i^h, \tag{59}$$

where ϑ_i^h is the angle between stress axis and the normal to the habit plane, where the new phase appears. Then the mechanical contribution of the free energy change can be decomposed into the tangential and normal part:

$$\begin{aligned}
\Delta G_\sigma^{mic} &= \frac{A^{hab}}{Vmic}\left(\Delta G_{\tau\sigma}^{mic} + \Delta G_{\sigma\sigma}^{mic}\right); \qquad (60)\\
\Delta G_{\tau\sigma}^{mic} &= \sum_{h=1}^{H}\left(\vec{\tau}^h \cdot \vec{\gamma}^h\right) = \frac{1}{2}\sum_{h=1}^{H}\left(\tau_i^h m_{ij}^h \gamma_j^h\right);\\
\Delta G_{\sigma\sigma}^{mic} &= \sum_{h=1}^{H}\left(\vec{\sigma}^h \cdot \vec{\epsilon}^h\right) = \frac{1}{2}\sum_{h=1}^{H}\sigma_i^h \epsilon_i^h
\end{aligned}$$

with vector product $\bullet$, the normal displacement ϵ_i^h, the tangent displacement (shear) γ_i^h. The directional tensor m_{ij}^h is defined by

$$m_{ij}^h = cos\zeta_{ij}^h, \tag{61}$$

where ζ_{ij}^h is the angle between the transformation tangent displacement $\vec{\gamma}^h$ and $\vec{\tau}^h$ direction.

A particular value of ΔG_σ^{mic} varies between the minimum and maximum value, i.e.

$$\Delta G_\sigma^{min} < \Delta G_\sigma^{mic} < \Delta G_\sigma^{max} \tag{62}$$

with

$$\begin{aligned}
\Delta G_\sigma^{min} &= -\frac{1}{2}\sum_{h=1}^{H}(-\tau_i^h s_i^{h_0} + \sigma_i^h \epsilon_i^h);\\
\Delta G_\sigma^{max} &= -\frac{1}{2}\sum_{h=1}^{H}(\tau_i^h s_i^{h_0} + \sigma_i^h \epsilon_i^h), \qquad (63)
\end{aligned}$$

where $s_i^{h_0}$ is the transformation tangent displacement parallel with the shear stress vector resolved on the habit plane.

When deformation is controlled by stress coupled with phase transformation, experimental results available for a one-dimensional test [9] show the linear relation between the martensite fraction $\hat{y}_6$ and the resulting plastic strain $\bar{E}^p$. This originally has been used in [39] to propose a kinetic equation suitable for one-dimensional microregion. The newly proposed three-dimensional generalization of this evolution law has been obtained by using Eq.(55) in Eq.(57), and substituting the resultant relation to Eq.(53). This generalized kinetic equation is written in the form:

$$\hat{y}_6 = \frac{\bar{E}^p}{\bar{E}_1} = 1 - \exp[-V^{mic} N_V(\mathcal{G}_\sigma)], \tag{64}$$

where $\bar{E}^p = (\frac{4}{3} I_{E^p})^{\frac{1}{2}}$ is the effective plastic strain, and $\bar{E}_1 = (\frac{4}{3} I_E)^{\frac{1}{2}}$ is the effective total strain for the fully martensitic structure of a microregion when $y_6 = 1$. Assuming $\mathcal{G}_\sigma = \mathcal{G}_\sigma^{min}$ and splitting the integral in Eq.(57) into two

$$\int_{\mathcal{G}_\sigma^{min}}^{\mathcal{G}_\sigma^{max}} ...d\mathcal{G} = \int_0^{\mathcal{G}_\sigma^{max}} ...d\mathcal{G} - \int_0^{\mathcal{G}_\sigma^{min}} ...d\mathcal{G}, \tag{65}$$

the nucleation-site potency N_V can be expressed as

$$N_V = \mathcal{I}_{max} - \mathcal{I}_{min}. \tag{66}$$

Integrals $\mathcal{I}_{min}$, $\mathcal{I}_{max}$ are defined by

$$\mathcal{I}_{min}(\mathcal{G}_\sigma^{min}) = \int_0^{\mathcal{G}_\sigma^{min}} M(\mathcal{G})\exp\left(\frac{L}{D_1}\right) d\mathcal{G}; \tag{67}$$

$$\mathcal{I}_{max}(\mathcal{G}_\sigma^{max}) = \int_0^{\mathcal{G}_\sigma^{max}} M(\mathcal{G})\exp\left(\frac{L}{D_2}\right) d\mathcal{G}; \tag{68}$$

$$\begin{aligned}
&D_1 = (A_6^{mic}\gamma_6 - \Delta G_{ch_6}^{mic} + \Delta G_F^{mic})d_6\\
&D_2 = D_1 + \mathcal{G}_\sigma d_6\\
&L = 2\ \alpha\ \gamma_6;\\
&\mathcal{G}_\sigma^{min} = \Delta G_\sigma^{min}\ ; \mathcal{G}_\sigma^{max} = \Delta G_\sigma^{max};\\
&d\mathcal{G} = d(\Delta G_\sigma^{mic}).
\end{aligned}$$

Substituting Eq.(66) into Eq.(64) results in

$$\hat{y}_6 = 1 - \exp[-V^{mic}(\mathcal{I}_{max} - \mathcal{I}_{min})]. \tag{69}$$

Estimated values of the following quantities: $\alpha = 0.84$, $N_V^0 = 2.0E+17\ [m^{-3}]$, $\gamma_6 = 0.15\ [J/m^2]$, $A_6^{mic}\gamma_6 + \Delta G_F^{mic} = 6.1E+7\ [J/m^3]$, can be found in [11] and [39].

A simpler model is obtained by postulating the structural defect potency as a function of $\mathcal{G}_\sigma$ and G in the following form:

$$\begin{aligned}
&N_V = N_V^0(\mathcal{G}_\sigma)\ \exp(G); \qquad (70)\\
&G = \frac{2\alpha\gamma_6}{d_6\left(A_6^{mic}\gamma_6 - \Delta G_{ch_6}^{mic} + \mathcal{G}_\sigma^{max} + \Delta G_F^{mic}\right)}.
\end{aligned}$$

Then the martensitic fraction can be defined by

$$\hat{y}_6 = 1 - \exp\left[-V^{mic} N_V^0(\mathcal{G}_\sigma)\ \exp(G)\right]. \tag{71}$$

Assuming $n = \mathcal{N}(\mathcal{G}_\sigma, \theta)$ in Eq.(53) results in

$$\ln(1 - \hat{y}_6) = -V^{mic} N_V\ (\mathcal{G}_\sigma, \theta) \tag{72}$$

which after differentiation in respect of time is written as

$$\frac{\dot{\hat{y}}_6}{1 - \hat{y}_6} = V^{mic}\left(\frac{\partial N_V}{\partial \mathcal{G}_\sigma}\dot{\mathcal{G}}_\sigma + \frac{\partial N_V}{\partial \mathcal{G}_{ch}}\frac{d\mathcal{G}_{ch}}{d\theta}\dot{\theta}\right) \tag{73}$$

where

$$\mathcal{G}_\sigma = \Delta G_\sigma^{mic};\ \mathcal{G}_{ch} = \Delta G_{ch_6}^{mic}. \tag{74}$$

Partial derivatives of N_V can be eliminated using Eqs.(54), (55) and assuming N_V^0 as a function of $\mathcal{G}$.

The final form of the evolution equation derived from thermodynamics and statistical analysis follows:

$$\begin{aligned}
&\frac{\dot{\hat{y}}_6}{1-\hat{y}_6} = V^{mic}\exp\left(\frac{-2\alpha\gamma_6}{M}\right)\times \\
&\left[\left(\frac{dN_V^0}{d\mathcal{G}_\sigma} - P_1\right)\dot{\mathcal{G}}_\sigma + P_1\frac{d\mathcal{G}_{ch}}{d\theta}\dot{\theta}\right]; \\
&\mathcal{G}_{AF} = A_6^{mic}\gamma_6 + \Delta G_F^{mic}; \\
&M = d_6(\mathcal{G}_{AF} - \mathcal{G}_{ch} + \mathcal{G}_\sigma); \\
&P_1 = N_V^0\frac{2d_6\alpha\gamma_6}{M^2}.
\end{aligned} \tag{75}$$

Unfortunately replacing Eq.(57) by Eq.(54) eliminates the coupling effect between N_V and $\mathcal{G}_\sigma$ expressed by the integration of $M(\mathcal{G})$ at the range of the mechanical contribution of the free energy change.

A simpler evolution equation is obtained from Eq.(71) in the form

$$\begin{aligned}
&\frac{\dot{\hat{y}}_6}{1-\hat{y}_6} = V^{mic}\exp\left(\frac{-2\alpha\,\gamma_6}{M}\right)\times \\
&\left[\frac{dN_V^0}{d\mathcal{G}_\sigma}\dot{\mathcal{G}}_\sigma + P_1\frac{d\mathcal{G}_{ch}}{d\theta}\dot{\theta}\right],
\end{aligned} \tag{76}$$

where $\mathcal{G}_\sigma$ is replaced by $\mathcal{G}_\sigma^{max}$ in M.

3.3.3 Kinetic Equations Derived from Thermodynamics

Growth laws developed on the basis of thermodynamics of continua and micromechanics have been presented in [38] and [50]. Both of them are based on the following observations:

- a volume average of the total driving force, $\langle d\Delta G_6^{mic}\rangle$, together with temperature θ controls the martensitic transformation,
- the macroscopic increment of the daughter phase dy_6 is proportional to the increment of the total driving force.

These notions are used to express the fraction y_6 as a function of temperature θ and external loading stress $\mathcal{S}$, such as $y_6 = \mathcal{Y}_1[\tilde{\mathbf{S}}(\mathcal{S}),\theta] = \mathcal{Y}_2(\mathcal{S},\theta)$.

In this section a kinetic law, originally shown in [38] for the case when the growth of martensitic fraction is the only reaction, is slightly generalized to be used for a description of transformation occuring in the presence of products of diffusional transformations y_2, y_3, y_4 and y_5.

The proportional relation between a phase fraction and the driving force is expressed here in terms of $d\hat{y}_6$ and $d\mathcal{G}$, and is written in the form:

$$\begin{aligned}
\frac{d\hat{y}_6}{\langle d\mathcal{G}\rangle} &= -k_F V^{mic}(1-\hat{y}_6); \\
\mathcal{G} &\equiv \mathcal{G}(\tilde{\mathbf{S}},\theta) = \Delta G_6^{mic}(\tilde{\mathbf{S}},\theta),
\end{aligned} \tag{77}$$

where $\tilde{\mathbf{S}}$ is the total stress related linearly to $\mathcal{S}$, V^{mic} is the microregion volume average, $\langle\Delta G_6^{mic}\rangle$ is the volume average of ΔG_6^{mic} taken for the parent phase, and k_F is a constant given for steel in [38] as $k_F V^{mic} = 0.0206\ m^2/N$.

Eq.(77), as all previously reviewed kinetic equations, is subjected to another assumption about the exponential form of the function $\hat{y}_6 = \mathcal{Y}_1(\tilde{\mathbf{S}},\theta)$. This becomes obvious due to the following transformations:

- move all terms with $\hat{y}_6$ to the left

$$\frac{d\hat{y}_6}{1-\hat{y}_6} = -k_F V^{mic}\langle d\mathcal{G}\rangle, \tag{78}$$

- integrate

$$\ln(1-\hat{y}_6) = k_F V^{mic}\langle\mathcal{G}\rangle + \mathcal{C}, \tag{79}$$

- express Eq.(79) in the exponential form

$$\begin{aligned}
\hat{y}_6 &\equiv \mathcal{Y}_1(\tilde{\mathbf{S}},\theta) \\
&= 1-\exp\left[k_F V^{mic}\langle\mathcal{G}(\tilde{\mathbf{S}},\theta)\rangle + \mathcal{C}\right],
\end{aligned} \tag{80}$$

with the integration constant $\mathcal{C}$,

- assume $\mathcal{C}$ equal to zero.

Eq.(80) reveals the interaction between the martensitic transformation product $\hat{y}_6$, the total stress $\tilde{\mathbf{S}}$, and temperature θ.

The required function $\hat{y}_6 = \mathcal{Y}_2(\mathcal{S},\theta)$ is derived by considering chemical and mechanical components of the total Gibbs free energy. The total driving force can be represented by a difference of mechanical and chemical components of the total Gibbs free energy:

$$\Delta G_6^{mic} = \Delta G_\sigma^{mic} - \Delta G_{ch}^{mic} \tag{81}$$

when neglecting frictional effects on habit planes ΔG_F^{mic} and the elastic coherency interfacial energy $A_6^{mic}\gamma_6$ in Eq.(56). The strain energy is given by

$$\Delta G_\sigma^{mic} = \tilde{\mathbf{S}} : \mathbf{E}^*. \tag{82}$$

The chemical free energy is derived using Eqs.(7), (8), and is defined by

$$\begin{aligned}
\Delta G_{ch}^{mic} &= \sum_{l=1}^{\mathcal{N}(t)} V_l^{nuc}\Delta G_{ch_6} \\
&= \sum_{l=1}^{\mathcal{N}(t)} a_l^2 c_l \Delta G_{ch_6},
\end{aligned} \tag{83}$$

where $\mathbf{E}^*$ is the microscopic transformation strain, and $\mathcal{N}(t)$ is the time related number of nuclei in a microregion. The strain $\mathbf{E}^*$ is measured in the stress free state as a difference of strains before and after phase transformation.

The total stress $\tilde{\mathbf{S}}$ in Eq.(82) is a sum of the following components:

- an actually self-equilibrating stress $\tilde{\mathbf{S}}_{eq}^{act}$,
- a further generated self-equilibrating stress $\tilde{\mathbf{S}}_{eq}^{fur}$,
- the loading external stress $\mathcal{S}$ assumed to be homogeneous in the mesodomain.

The actually self-equilibrating stress reveals the interaction of all actually transformed microregions with the microregion under consideration. The further self-equilibrating stress is generated by the interaction of the microregion which undergoes transformation and the surrounding mesodomain. The load stress is assumed to be homogeneous in the mesodomain. This stress distribution can be written as

$$\tilde{\mathbf{S}} = \tilde{\mathbf{S}}_{eq}^{act} + \tilde{\mathbf{S}}_{eq}^{fur} + \mathcal{S}. \tag{84}$$

Substituting Eq.(84) in Eq.(82) results in

$$\begin{aligned} &\Delta G_{\sigma}^{mic}(\mathbf{S}) \equiv \Delta G_{\sigma}^{mic}(\mathcal{S}, \tilde{\mathbf{S}}_{eq}^{act}, \tilde{\mathbf{S}}_{eq}^{fur}) \\ &= \tilde{\mathbf{S}}_{eq}^{act} : \mathbf{E}^* + \tilde{\mathbf{S}}_{eq}^{fur} : \mathbf{E}^* + \mathcal{S} : \mathbf{E}^*. \end{aligned} \tag{85}$$

The total differential of $\Delta G_{\sigma}^{mic}(\mathcal{S}, \tilde{\mathbf{S}}_{eq}^{act}, \tilde{\mathbf{S}}_{eq}^{fur})$ with respect of $\tilde{\mathbf{S}}$ components is given as

$$d\Delta G_{\sigma}^{mic} = d\tilde{\mathbf{S}}_{eq}^{act} : \mathbf{E}^* + d\tilde{\mathbf{S}}_{eq}^{fur} : \mathbf{E}^* + d\mathcal{S} : \mathbf{E}^*. \tag{86}$$

Substituting Eq.(86) in Eq.(81) and averaging $d\Delta G_6^{mic}$ over volume gives

$$\begin{aligned} \langle d\mathcal{G} \rangle \equiv\ & \langle d\Delta G_{\sigma}^{mic} \rangle - \langle d\Delta G_{ch}^{mic} \rangle \\ =\ & \langle d\tilde{\mathbf{S}}_{eq}^{act} : \mathbf{E}^* \rangle + \langle d\tilde{\mathbf{S}}_{eq}^{fur} : \mathbf{E}^* \rangle \\ & \langle d\mathcal{S} : \mathbf{E}^* \rangle - \langle d\Delta G_{ch}^{mic} \rangle. \end{aligned} \tag{87}$$

The volume average of work done by the external stress $\mathcal{S}$ on the microscopic strain $\mathbf{E}^*$ is replaced by the contraction of $\mathcal{S}$ and the volume average of $\mathbf{E}^*$, which is expressed by

$$\langle d\mathcal{S} : \mathbf{E}^* \rangle = d\mathcal{S} : \langle \mathbf{E}^* \rangle. \tag{88}$$

This replacement can be done because at the start of transformation, $\hat{y}_6 \ll 1$, the martensitic inclusions are oriented "optimally" in respect to $\mathcal{S}$ and when the transformation develops, internal stress increases and martensitic microregions get less favourable orientation [38]. Substituting Eq.(87) and Eq.(88) in Eq.(78) gives

$$\begin{aligned} &\frac{d\hat{y}_6}{1-\hat{y}_6} = -\, k_F V^{mic} \\ &\times \Big[\langle d\tilde{\mathbf{S}}_{eq}^{act} : \mathbf{E}^* \rangle + \langle d\tilde{\mathbf{S}}_{eq}^{fur} : \mathbf{E}^* \rangle \\ &+ d\mathcal{S} : \langle \mathbf{E}^* \rangle - \langle d\Delta G_{ch}^{mic} \rangle \Big]. \end{aligned} \tag{89}$$

Rearranging of Eq.(89) by shifting the first two RHS terms, which are evidently related to the progress of martensitic transformation and $\hat{y}_6$, to the LHS results in

$$\begin{aligned} &\Big[\frac{1}{1-\hat{y}_6} + k_F V^{mic} \langle \frac{d\tilde{\mathbf{S}}_{eq}^{fur}}{d\hat{y}_6} : \mathbf{E}^* \rangle \\ &+ k_F V^{mic} \langle \frac{d\tilde{\mathbf{S}}_{eq}^{act}}{d\hat{y}_6} : \mathbf{E}^* \rangle \Big] d\hat{y}_6 \\ =\ & k_F V^{mic} \langle \frac{d\Delta G_{ch}^{mic}}{d\theta} \rangle d\theta \\ -\ & k_F V^{mic} \langle \mathbf{E}^* \rangle : d\mathcal{S}. \end{aligned} \tag{90}$$

Considering $\hat{y}_6$, temperature θ, and external stress $\mathcal{S}$ as time dependent functions, the kinetic equation given as Eq.(90) can be written as the evolution equation

$$\begin{aligned} &\Big[\frac{1}{1-\hat{y}_6} + k_F V^{mic} \langle \frac{d\tilde{\mathbf{S}}_{eq}^{fur}}{d\hat{y}_6} : \mathbf{E}^* \rangle \\ &+ k_F V^{mic} \langle \frac{d\tilde{\mathbf{S}}_{eq}^{act}}{d\hat{y}_6} : \mathbf{E}^* \rangle \Big] \dot{y}_6 \\ =\ & k_F V^{mic} \langle \frac{d\Delta G_{ch}^{mic}}{d\theta} \rangle \dot{\theta} \\ -\ & k_F V^{mic} \langle \mathbf{E}^* \rangle : \dot{\mathcal{S}}. \end{aligned} \tag{91}$$

The simple form of the above evolution equation is obtained due to the following operations and assumptions:

- The third term of LHS of Eq.(91) can be expressed by

$$\begin{aligned} &\langle \frac{d\tilde{\mathbf{S}}_{eq}^{act}}{d\hat{y}_6} : \mathbf{E}^* \rangle = -p \frac{d\mathcal{F}}{d\hat{y}_6} \langle \mathbf{I} : \mathbf{E}^* \rangle \\ =\ & -2p\, \hat{y}_6\, \mathrm{tr}\mathbf{E}^*, \end{aligned} \tag{92}$$

  when the stress $\tilde{\mathbf{S}}_{eq}^{act}$ is substituted by $-(p\mathcal{F}(\hat{y}_6)\mathbf{I})$, and the function $\mathcal{F}(\hat{y}_6)$ is assumed to be the quadratic one i.e. $\mathcal{F}(\hat{y}_6) = \hat{y}_6^2$. The average final hydrostatic stress at $y_6 = 1$ is p, and $\mathbf{I}$ is the unit second order tensor.

- The second term of RHS of Eq.(91) can be replaced by

$$k_F V^{mic} \langle \mathbf{E}^* \rangle : \dot{\mathcal{S}} = k_F V^{mic} \hat{y}_6^{\frac{1}{n}}\, \mathbf{E}_{cr}^* : \dot{\mathcal{S}}, \tag{93}$$

with $\mathbf{E}^*_{cr}$ being $\mathbf{E}^*$ when $y_6 = 1$ and the entire microregion transforms to martensite, and the exponent $n > 1$. This replacement reflects a decrease of deformation and $\frac{d\mathbf{E}^*}{d\hat{y}_6}$ due to the internal stress increase during transformation.

- The term with $\tilde{\mathbf{S}}^{fur}_{eq}$ in Eq.(91) can be neglected because its influence is indirectly accounted for by evaluation of thermo-elastic stresses. This assumption follows the Eshelby concept presented in [14] and utilised previously in [50].

The simplified evolution equation for the martensitic transformation has the form

$$\begin{aligned} &\left(\frac{1}{1-\hat{y}_6} - 2k_F V^{mic} p\, \hat{y}_6\, \mathrm{tr}\mathbf{E}^*\right)\dot{\hat{y}}_6 \\ = \quad & k_F V^{mic}\langle\frac{d\Delta G^{mic}_{ch}}{d\theta}\rangle\dot{\theta} \\ - \quad & k_F V^{mic}\hat{y}_6^{\frac{1}{n}}\,\mathbf{E}^*_{cr} : \dot{\mathcal{S}}. \end{aligned} \tag{94}$$

The solution of Eq.(91) and/or Eq.(94) is the function $\mathcal{Y}_2(\mathcal{S}, \theta)$ which determines the martensitic volume fraction $\hat{y}_6$ as a function of the external load stress $\mathcal{S}$ and temperature θ.

Parameters of evolution equation Eq.(94) have the following values given in [38]: $k_F V^{mic}$ equals to $0.0206\ m^2/N$, hydrostatic pressure p ranges from 0 to 50 MPa, the first invariant of strain tensor $\frac{1}{3}\mathrm{tr}\mathbf{E}^*$ is equal to 0.04, $[k_F V^{mic}(\frac{d\Delta G^{mic}_c}{d\theta})] = 0.0484°C^{-1}$, the microscopic transformation strain $\mathbf{E}^*$ at the stress-free state is ranging from 0.07 to 0.29.

4. Approximation of Cooling Process

The growth law for incomplete diffusional reactions Eq.(30) together with the law for bainitic transformation, and one of the equations describing the martensitic transformation, the Scheil sum, and the additivity principle are essential notions for the incremental evaluation of the material composition and determination of nonhomogeneous material functions which are stress, temperature and time dependent.

4.1 Approximation of Cooling Curve

An incremental analysis of thermo-mechanical-metallurgical problem requires an approximation of a continuous cooling process, which describes temperature changes in a microregion and is called the cooling rule. The cooling process is replaced by a sequence of isothermal processes due to the additivity principle for incubation fractions, proposed by Scheil [47]. Hence, the cooling process $\theta(t)$, can be approximated by a stepped-function with isothermal "steps" ${}^i\theta$. Each isothermal step-process lasts $\Delta^i t^{cp}$ and starts at ${}^i t$.

A transformation time for approximated cooling process is separated into the nucleation period and the growth period. The growth period of a phase transformation starts when a graph representing cooling process intersects the TTT (Time- Temperature-Transformation) curve which is determined either by dilatometric or thermal analysis for a particular welded steel. The incubation period delays the daughter phase growth and terminates, when the Scheil sum is equal to unity. This requirement can be written in the form

$$\sum_{i=1}^{s} \frac{\Delta^i t^{cp}}{{}^i Z^{TTT}} = 1, \tag{95}$$

which is related to two graphs: a curve representing a cooling process, and one of curves of the TTT diagram. The length $\Delta^i t^{cp}$ of temperature step ${}^i\theta$ results from the step-approximation of a cooling curve, and ${}^i Z^{TTT}$ is time measured on the TTT curve which corresponds to the same temperature ${}^i\theta$. Pairs $\{{}^i\theta, {}^i Z^{TTT}\}$ determine points of the TTT curve. The pair $\{{}^s\theta, {}^s t\}$ represent a point of intersection of a particular cooling curve and one of the TTT curves. The growth period starts at time ${}^s t$, and temperature ${}^s\theta$ corresponds to this moment of time.

4.2 Approximation of TTT Diagram

Each curve of the TTT diagram is approximated by a sequence of piecewise straight lines and saved in a computer program in the form of two columns matrix. Intersections of a cooling curve with one of the TTT branches can be found numerically using one of the searching procedures.

4.3 Schemes for Approximation of Transformation Sequence

Assuming that material state variables: $\mathbf{S}$, $\mathbf{E}$, and θ are known, and diffusional transformations are followed by diffusionless transformations, when decreasing temperature reaches values either W_s or M_s, **two numerical schemes** can be proposed for evaluation of material phase fractions y_i.

The first scheme is suitable for the modified Johnson- Avrami- Mehl evolution equation Eq.(31), the evolution equation for bainitic transformation Eq.(37), and the extended Koistinen-Marburger law given by Eq.(49). Time is not involved explicitly in the last two equations. The Johnson-Avrami-Mehl law expressed by Eq.(30), is the basis for evaluation of the fictitious time ${}^j t^\phi$ related to the fictitious fraction ${}^j y^\phi$. The fictitious time for the isothermal transformation at temperature ${}^j\theta$ is given by

$${}^j t^\phi = \left(\frac{-\ln(1 - {}^j y_i^\phi)}{{}^j b_{D_i}}\right)^{1/m(j)}, \tag{96}$$

where ${}^{j}b_{D_i}$ and $m(j) = {}^{j}n_i$ are growth parameters taken at j-th time step.

Knowing the fictitious time ${}^{j}t^{\phi}$ at the end of j-step of an isothermal process, the fictitious phase fraction y_i^{ϕ} at $(j+1)$-th time instant is evaluated from the equation, such that

$$\dot{y}_i^{\phi} \equiv \mathcal{F}(\tau, y_i^{\phi}) = {}^{j}\mathcal{A}\,\tau^{n_i}\left({}^{j}\mathcal{B}\,{}^{j}\dot{\theta} + {}^{j}\mathcal{C}\,{}^{j}\dot{\mathbf{S}} + {}^{j}\mathcal{D}\right)(1-y_i^{\phi}), \quad (97)$$

which is obtained from Eq.(31) substituting the following notations:

$${}^{j}\mathcal{A} = (1 - C\,{}^{j}J_2')^{-n_i};$$

$${}^{j}\mathcal{B} = \frac{db_i}{d\theta}\Big|_{{}^{j}t^{\phi}};$$

$${}^{j}\mathcal{C} = \frac{b_i({}^{j}\theta)n_i C}{1 - C\,{}^{j}J_2'}\,\frac{dJ_2'}{d\mathbf{S}}\Big|_{{}^{j}t^{\phi}};$$

$${}^{j}\mathcal{D} = \frac{b_i({}^{j}\theta)n_i}{{}^{j}t^{\phi}}.$$

This evolution equation is valid for time τ taken at the interval $[{}^{j}t^{\phi}, ({}^{j}t^{\phi} + \Delta^{j}t)]$.

The fourth order Runge-Kutta method is applied to solve Eq.(97) for ${}^{(j+1)}y_i^{\phi}$. Phase fraction ${}^{(j+1)}y_i$ can be found from

$${}^{(j+1)}y_i = {}^{(j+1)}y_i^{\phi}\; y_{\gamma}\; y_{i_{max}}. \quad (98)$$

Diffusional -pearlitic transformation terminates when temperature ${}^{j}\theta$ reaches the Widmanstatten temperature W_s, and the bainitic transformation starts. The bainitic volume fraction can be calculated from the algebraic expression which is obtained from Eq.(38) due to linearization of terms related to y_4^{ϕ}. Such a formula is written as

$${}^{j}y_4^{\phi} = 1 - \exp\left[\frac{1}{{}^{j}A}\times\left({}^{j}\mathcal{B} + {}^{j}\mathcal{C} - \frac{{}^{j}t_b\;{}^{j}M\left(\mathcal{G}^0, \frac{1}{\theta}\right)}{\gamma}\right)\right]; \quad (99)$$

$${}^{j}\mathcal{B} = \frac{{}^{j}B}{\gamma\,\beta}\ln\left(1 - \beta\,\gamma\;{}^{(j-1)}y_4^{\phi}\right);$$

$${}^{j}\mathcal{C} = \frac{{}^{j}C}{\langle {}^{j}\Gamma_2\rangle}\left(1 - \mathrm{e}^{-\langle {}^{j}\Gamma_2\rangle\;{}^{(j-1)}y_4^{\phi}}\right).$$

where time t_b is calculated from the beginning of the bainitic transformation.

The bainitic transformation terminates when temperature ${}^{j}\theta$ reaches value M_s. Then the martensitic transformation starts and ${}^{j}\hat{y}_6$ is calculated from the extended Koistinen- Marburger Eq.(49)

$${}^{j}\hat{y}_6 = \{1 - \exp[-\alpha(M_s + {}^{j}\Delta M_s - {}^{j}\theta)]\}; \quad (100)$$

$${}^{j}\Delta M_s = A\,{}^{j}p + B\,{}^{j}\hat{\mathbf{S}},$$

where time is not involved directly and $\hat{y}_6$ is coupled with temperature, internal pressure and stress state.

The second scheme is obtained by replacing parabolic exponential law, expressed in the form of Eq.(49), by the simplified evolution equation for the martensitic transformation written as Eq.(94). The evolution equation for $\hat{y}_6$ can be expressed by

$$\dot{\hat{y}}_6 = \mathcal{A}(1-\hat{y}_6)\left(\mathcal{B} : \dot{\mathcal{S}} - \mathcal{C}\,\dot{\theta}\right), \quad (101)$$

$$\mathcal{A} = \left[1 + 2k_F V^{mic} p\,\hat{y}_6(1-\hat{y}_6)\mathrm{tr}\mathbf{E}^*\right]^{-1}$$

$$\mathcal{B} = k_F V^{mic}\hat{y}_6^{\frac{1}{n}}\,\mathbf{E}_{cr}^*$$

$$\mathcal{C} = k_F V^{mic}\frac{d\Delta G_{ch}^{mic}}{d\theta}.$$

Unfortunately, time is represented here implicitly via functions, such as: $\mathcal{S}(t), \mathbf{E}^*(t), p(t), \theta(t), \hat{y}_6(t)$. This results from the fact that time, in contradiction to stress, elastic strain, internal pressure and temperature, is not a physical quantity which is controlling the martensitic transformation. Hence, time t_m of martensitic transformation can be introduced explicitly due to the purely analytical approximation which is provided by the following identification:

$$\mathcal{B} : \dot{\mathcal{S}} - \mathcal{C}\,\dot{\theta} \equiv \frac{3}{2}\,a\,t_m^{\frac{1}{2}} + b. \quad (102)$$

Parameters of this identity are deduced verifying relations shown in [38], and they are given by

$$a = -\left\{\frac{4}{9}\left[1 - \exp\left(\frac{b^3}{a^2} - \frac{3}{2}\right)\right]\mathcal{B} : \dot{\mathcal{S}}\right\}^{\frac{3}{2}};$$

$$b = \mathcal{C}\,\dot{\theta}.$$

Substituting Eq.(102) in Eq.(101), the evolution equation for the martensitic transformation can be written in the form, where reaction time is represented explicitly. The equation has the following form:

$$\dot{\hat{y}}_6 \equiv \mathcal{F}(\tau, \hat{y}_6) = {}^{j}\mathcal{A}\left(\frac{3}{2}\,{}^{j}a\tau^{\frac{1}{2}} + {}^{j}b\right)\times(1-\hat{y}_6), \quad (103)$$

where

$${}^{j}\mathcal{A} = \left[1 + 2k_F V^{mic}\,{}^{j}p\,{}^{j}\hat{y}_6(1-{}^{j}\hat{y}_6)\mathrm{tr}\{{}^{j}\mathbf{E}^*\}\right]^{-1};$$

$${}^{j}a = -\left\{\frac{4}{9}\left[1 - \exp\left(\frac{{}^{j}b^3}{{}^{j}a^2} - \frac{3}{2}\right)\right]{}^{j}\mathcal{B} : {}^{j}\dot{\mathcal{S}}\right\}^{\frac{3}{2}};$$

$${}^{j}b = {}^{j}\mathcal{C}\,{}^{j}\dot{\theta};$$

$${}^{j}\mathcal{B} = k_F V^{mic}\,{}^{j}\hat{y}_6^{\frac{1}{n}}\,{}^{j}\mathbf{E}_{cr}^*;$$

$${}^{j}\mathcal{C} = k_F V^{mic}\frac{d\Delta G_{ch}^{mic}}{d\theta}\Big|_{{}^{j}t_m}.$$

Time τ is taken at the interval $[{}^{j}t_m, ({}^{j}t_m + \Delta^{j}t_m)]$. The fourth order Runge-Kutta method can also be applied to solve Eq.(103) for ${}^{(j+1)}y_6$.

Table 1 Basic assumptions for modeling of diffusional and diffusionless transformations. The following abbreviations and symbols are used in the table: JAM: Johnson -Avrami -Mehl, KM: Koistinen -Marburger, OTC: Olson -Tsuzaki -Cohen, OFT: Oberaigner -Fisher -Tanaka, RB: Rees -Bhadeshia, $\propto$: proportionality symbol.

Model	Assumption:		proportion of increments
JAM Eq.(14)	dy_i	$\propto$	$d\mathcal{G}$
	$\dot{\mathcal{G}}$	$\equiv$	$n_i b_i t^{n_i-1}$
JAM Eq.(24)	dy_i^ϕ	$\propto$	$d\mathcal{G}$
	$\dot{\mathcal{G}}$	$\equiv$	$n_i\ b_i\ t^{n_i-1}$
modified JAM Eq.(31)	dy_i^ϕ	$\propto$	$d\mathcal{G}, d\mathbf{S}, d\theta$
RB Eq.(32)	dy_4^ϕ	$\propto$	$\langle dN_4 \rangle$
KM Eq.(46)	$d\hat{y}_6$	$\propto$	$d\theta$
extended KM Eq.(49)	$d\hat{y}_6$	$\propto$	$d\theta, dp$, equivalent stress $d\hat{\mathbf{S}}$
OTC Eq.(53)	$d\hat{y}_6$	$\propto$	structural defect potency $dN_V(\mathcal{G}_\sigma)$
OFT Eq.(78)	$d\hat{y}_6$	$\propto$	total Gibbs free energy $\langle d\Delta G_6^{mic} \rangle$

Table 2 Microscopic and macroscopic variables of phase transformation models.

Model	Level of model variables	
	microscopic	macroscopic
JAM Eq.(14)		n_i, b_i
JAM Eq.(24)	$N_i(\theta)$	θ, n_i
modified JAM Eq.(31)		C, n_i, $b_i(\theta)$, J_2', θ
RB Eq.(33)		N_4
RB Eq.(37)		$\Delta G_{4_{max}}, G_N, \theta$ K_1, K_2, β, r, R
KM Eq.(46)		θ, α, M_s
extended KM Eq.(49)		A, B, α, θ, p, $\hat{S}$
OTC Eq.(75) or Eq.(76)	d_6,A_6^{mic}, ΔG_F^{mic} N_V^0,$\mathcal{G}_\sigma$, $\mathcal{G}_{ch}$,	θ, α, γ_6
OFT Eq.(78)	ΔG_{ch}^{mic}	k_F, $tr\mathbf{E}^*$, $\mathbf{E}_{cr}^*$, θ, p, $\mathcal{S}$

5. Conclusions

A unified mathematical approach has been applied to several phase growth laws to derive corresponding evolution equations from basic postulate of proportionality of the new phase increment to a change of a physical quantity controlling the transformation process. Table(1) contains a tabulation of basic assumptions for the kinetic laws reviewed.

Evolution laws reveal interactions between transformation kinetics and material constitutive variables or phase transformation driving forces. These equations are consistent with the rate type balance laws for conservation of virtual and internal energy. In thermo-mechanical-metallurgical analysis, constitutive variables are defined at a dispersed material particle. Material parameters and physical quantities are averaged proportionally to a phase fraction according to the linear averaging rule. A condensed presentation of features of nine models is given in Table(2) and Table(3) which helps in drawing conclusions on complexity of evolution equations, measurability of model variables, application, and required level of model variables. The simplest evolution laws for diffusional and diffusionless transformations expressed by Eq.(26) and Eq.(47) respectively, reveal only a relation between $\dot{\mathbf{y}}$ and temperature rate $\dot{\theta}$. Also they provide comparatively easy identification of material and process characteristics. The evolution law deduced in [39] from thermodynamics and statistics for uniaxial loading has been generalized here for the three-dimensional case. This 3-D generalization, expressed by Eq.(75) or Eq.(76), together with the law derived from thermodynamics, and given by Eq.(91) or Eq.(94), provides the relation between the rate of martensitic fraction $\hat{y}_6$ and rates of strain energy ΔG_σ^{mic}, chemical energy $\Delta G_{ch_6}^{mic}$, and temperature θ. However they account for different scale effects in dispersed particle. The strain energy $\mathcal{G}_\sigma = \sum_{h=1}^{H} \left(\vec{\sigma}^h \bullet \vec{\epsilon}^h + \vec{\tau}^h \bullet \vec{\gamma}^h\right)$ in Eq.(75) is evaluated on the system of habit planes while the mechanical contribution of free energy change $\Delta G_\sigma^{mic}(\mathbf{S}, \tilde{\mathbf{S}}_{eq}^{act}, \tilde{\mathbf{S}}_{eq}^{fur}) = \tilde{\mathbf{S}}_{eq}^{act} : \mathbf{E}^* + \tilde{\mathbf{S}}_{eq}^{fur} : \mathbf{E}^* + \mathcal{S} : \mathbf{E}^*$ in Eq.(91) is defined as the value averaged for the entire microregion. The kinetic low expressed by Eq.(75) is less attractive than Eq.(91) because of the high cost of data acquisition from real experimental tests and rather limited observation of slips on habit planes. This also requires very small size of a microregion in analysis and can be used only in the case of micromechanics when the body has the diameter of a few grains. The kinetic low expressed by Eq.(75) is less attractive than Eq.(91) because of the high cost of data acquisition from real experimental tests and rather limited observation of slips on habit planes. This also requires very small size of a microregion in analysis and can be used only in the case of micromechanics when the body has the diameter of a few grains.

The generalized evolution equation for diffusionless-

Table 3 Evaluation of data acquisition, complexity and application of phase transformation model. Symbol: 1-to 3-D means that a transformation model can be applied for one-, two- and three-dimensional problems.

Model	complexity of equation	measurability of variables	application
JAM Eq.(14)	simple	easy	1- to 3-D
JAM Eq.(24)	simple	easy	1- to 3-D
modified JAM Eq.(31)	complex	expensive hard	1- to 3-D
RB Eq.(37)	complex	expensive easy	1- to 3-D
KM Eq.(46)	simple	easy	1- to 3-D
extended KM Eq.(49)	simple	expensive easy	1- to 3-D
OTC Eq.(75) or Eq.(76)	complex	generally impossible	1-D specific
OFT Eq.(78)	complex	hard	1- to 3-D

martensitic transformation is proposed in Table(4). Coefficients of this equation are identified for three kinetic laws: Eq.(47), Eq.(75), and Eq.(94). The generalized evolution equation for diffusional transformation is proposed in Table(5) with coefficients identified for Eq.(26) and its modification Eq.(26). Two numerical schemes have been postulated for the cooling part of welding process:

- the first is appropriate for the case when diffusional transformations are determined by evolution law, the bainitic reaction is governed by an algebraic equation, and time is not accounted directly in calculation of martensitic fraction,
- the second is proposed for the case when ferritic/pearlitic and martensitic growth laws are written in forms of evolution equations, Eqs.(97), (103), and where time is represented explicitly.

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Table 4 Generalized kinetic equations for diffusionless-martensitic transformation where $\dot{G}_\sigma$ is the mechanical contribution of Gibbs free energy.

The general form of kinetic low: $\dot{\hat{y}}_6 = \mathcal{L}(\mathbf{S}, \theta, \hat{y}_6, t)\dot{\theta} + \mathcal{K}(\mathbf{S}, \theta, \hat{y}_6, t)\dot{G}_\sigma$
KM Eq.(47)
$\mathcal{K}(\theta, \hat{y}_6, t) = 0$ $\mathcal{L}(\theta, \hat{y}_6, t) = \alpha(1 - \hat{y}_6)$
Newly proposed 3-D generalization of OTC expressed by Eq.(75)
$\mathcal{K}(\vec{\tau}, \vec{\sigma}, \theta, \hat{y}_6, t) = \mathcal{M}_1\mathcal{K}_1$ $\mathcal{K}_1 = \frac{dN_V^0}{d\mathcal{G}_\sigma} - P_1$ $\mathcal{L}(\vec{\tau}, \vec{\sigma}, \theta, \hat{y}_6, t) = \mathcal{M}_1\mathcal{L}_1$ $\mathcal{L}_1 = P_1 \frac{d\mathcal{G}_{ch}}{d\theta}$ $\mathcal{M}_1 = V^{mic} \exp\left(\frac{-2\alpha\gamma_6}{M}\right)(1 - \hat{y}_6)$ $\dot{G}_\sigma = \dot{\mathcal{G}}_\sigma$ given by Eq.(60)
OFT Eq.(94)
$\mathcal{K}(\mathbf{S}, \theta, \hat{y}_6, t) = \mathcal{M}_2\mathcal{K}_2$ $\mathcal{K}_2 = V^{mic} k_F \hat{y}_6 \frac{1}{n}$ $\mathcal{L} = \mathcal{M}_2\mathcal{L}_2$ $\mathcal{L}_2 = V^{mic} k_F \langle \frac{d\Delta G_{ch}^{mic}}{d\theta} \rangle$ $\mathcal{M}_2 = \left(\frac{1}{1-\hat{y}_6} - 2k_F V^{mic} p\ \hat{y}_6\ \mathrm{tr}\mathbf{E}^*\right)^{-1}$ $\dot{G}_\sigma = \mathbf{E}_{cr}^* : \dot{\mathcal{S}}$

Table 5 Generalized kinetic equation for diffusional transformation.

The general form of kinetic law: $\dot{y}_i^\phi = \mathcal{A}(\mathbf{S}, \theta, y_i^\phi, t)\dot{\theta} + \mathcal{B}(\mathbf{S}, \theta, y_i^\phi, t)\dot{\mathbf{S}} + \mathcal{R}(\mathbf{S}, \theta, y_i^\phi, t)$
JAM Eq.(26)
$\mathcal{A}(\theta, y_i, t) = t^{n_i} \frac{db_i}{d\theta}(1 - y_i^\phi)$; $\mathcal{B}(\theta, y_i, t) = 0$; $\mathcal{R}(\theta, y_i, t) = n_i b_i(\theta) t^{n_i - 1}(1 - y_i^\phi)$.
JAM Eq.(31)
$\mathcal{A}(\mathbf{S}, \theta, y_i, t) = \mathcal{N} \frac{db_i}{d\theta}(1 - y_i^\phi)$ $\mathcal{B}(\mathbf{S}, \theta, y_i, t) = \mathcal{N} \frac{b_i(\theta) C n_i}{1 - CJ_2'}(1 - y_i^\phi)$ $\mathcal{R}(\mathbf{S}, \theta, y_i, t) = \mathcal{N} \frac{b_i(\theta) n_i}{t}(1 - y_i^\phi)$ where $\mathcal{N} = \frac{t^{n_i}}{(1 - CJ_2')^{n_i}}$

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