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Thermo-Mechanical-Metallurgical Model of Welded Steel†

Part 2: Finite Element Formulation and Constitutive Equations

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Abstract

Papers that contribute to the phenomenological description of solid state transformations do not meet requirements of FE incremental formulation of thermo-mechanical-metallurgical problems. They are always inconsistent because the formulation of the mechanical problem is given in incremental form but phase evolution laws are given in algebraic form. Even when they are given in the evolution form, metallurgical phenomena are discoupled from thermo-mechanical variables.

Key words: (phase transformation), (thermo-mechanical-metallurgical problem), (evolution law), (temperature), (stress), (heat affected zone), (microregion), (Lagrangian description), (Galerkin type Finite Element Method), (Hilbert space), (Gateaux derivative), (singular surface), (ferritic), (pearlitic), (bainitic), (martensitic), (nucleation), (phase growth), (transformation plasticity), (consistent tangent modulus).

1. Introduction

This paper is an attempt to give the consistent formulation of coupled thermo-mechanical-metallurgical (TMM) problem treated as the generalization of thermo-mechanical (TM) problem. Such formulation can be shown in the form of partial differential equations—balance laws, and ordinary differential equations—microstructure evolution laws. The formulation of generalized TM process consists of phase transformation phenomena and ordinary thermo-mechanical process. The temperature, stresses and solid phase distribution in heat affected zone (HAZ) are state variables for TMM process. The fields of temperature, stress and strain are coupled with the material microstructure. The microstructure depends on the chemical composition of the steel and on its thermal and mechanical history. The state of stress and internal pressure affects the chain of subsequent transformations of the initial austenitic steel structure that undergoes four transformations: ferritic, pearlitic, bainitic, and martensitic. Mechanisms of phase transformation and evolution laws has been studied in [20].

The Lagrangian description of motion is used primarily when considering geometrically non-linear behaviour of inelastic materials since then the boundary conditions are usually referred to in the initial configuration.

The mathematical model of TMM process consists of three principles expressing the balance of momentum, the balance of internal energy, and the microstructure evolution law. The first principle can be written as the balance of virtual energy and the second after some transformations can be expressed as the heat equation for non-rigid conductor. The variational formulation of the coupled TM problem is given which is the basis for the finite element approximation.

The finite element method is applied to find the configuration of a finite number of material dispersed points called microregions. Each microregion is a super-element with uniform isobaric stress, and is composed of phases containing several elements.

Two global FE equations: one for TM problem, and the second for TMM problem are derived here.

Resulting nonlinear finite element system of equations is solved iteratively by the Newton-Raphson scheme.

2. Model of TMM Process

2.1 Lagrangian Description

The polycrystalline body is idealized by using the concept of a generalized material point representing a micro-region which is part of a grain deforming due to phase transformations without the restraints of the

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neighbouring parts of the body.

The stress inside the micro-region is averaged, and the strain and displacement are measured only at one or more particular points of the bounding surfaces where continuity conditions must be fulfilled for neighbouring regions. This concept allows one to treat the polycrystalline body motion as a continuum with internal local deformation of particles. It is also assumed that the shape of a micro-region does not vary significantly during a deformation process.

Lagrangian analysis is used with the initial position of the generalized particle $\mathbf{X}$ and the time t taken as independent variables. The variables (X_1^0, X_2^0, X_3^0) of $\mathbf{X}$ are global and called the Lagrangian or material variables. The internal deformation of the generalized particle is defined in terms of the local coordinate system. The local coordinate system can be transformed to the global one by using the orthogonal transformation matrix shown in [4].

The generalized particle is the smallest microstructural element of the alloy and can be imagined as the micro-region defined in [4] and [5] and seen to be like a point of the considered body. The definition of a micro-region and its deformation are developed from the concept of "free" deformation. This "free" deformation is defined with respect to a phase transformation and means the deformation to the extent when neither other micro-region nor the remaining part of the grain restrains the local deformation. For example, a micro-region for the martensitic transformation is a block of laths or a plate dependent on the form of martensitic precipitations. A group of micro-regions form a mesodomain and will be represented in FE analysis by a finite element.

The motion, which carries a fixed material element through various spatial positions, can be expressed by the function of motion $\mathbf{x} = \chi(\mathbf{X}, t)$. This function expressed in terms of Lagrangian variables, describe the variation of physical parameters for a given particle during its wandering through the space. The vector joining the point X and its actual position in the space $\mathbf{x} = (X_1^1, X_2^1, X_3^1)$ is the displacement vector given by $\mathbf{u} = \mathbf{X} - \mathbf{x}$. The constitutive variables i.e. the stress and strain measures used in the Lagrangian formulation are the second Piola-Kirchhoff stress and the Green-Lagrange strain which are energetically conjugated according to the Hill definition. The second Piola-Kirchhoff stress tensor $\tilde{\mathbf{S}}$ is given in terms of the Cauchy stress $\underline{\sigma}$ by the formula:

$$\tilde{\mathbf{S}} = \frac{\rho^0}{\rho^t} \mathbf{F}^{-1} \, \underline{\sigma} \, \{\mathbf{F}^{-1}\}^{\mathrm{T}} \tag{1}$$

where ρ^0, ρ^t are the reference and current densities, and the deformation gradient is

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}; \quad F_{iK} = x_{i,K} = \frac{\partial x_i}{\partial X_K}; \tag{2}$$

where $\mathbf{X}$ and $\mathbf{x} = \chi(\mathbf{X}, t)$ are the reference and current coordinates respectively. The Green-Lagrange strain conjugated with the second Piola-Kirchhoff stress is defined by:

$$\tilde{\mathbf{L}} = \frac{1}{2}(u_{I,J} + u_{J,I} + u_{K,I} u_{K,J}) \tag{3}$$

where the displacement gradient is

$$u_{I,J} = \frac{\partial u_I}{\partial X_J} \tag{4}$$

The large indices I, J, K refer to the reference configuration. The "," is the usual abbreviated notation for differentiation with respect to coordinates. Material parameters such as Young's modulus E, Poisson's ratio ν, yield limit, hardening parameters, thermal and others parameters of a mesodomain are evaluated by using the linear mixture rule that in vector form can be written as

$$\langle E \rangle = \underline{E} : \underline{y} \;, \; \langle \nu \rangle = \underline{\nu} : \underline{y} \tag{5}$$

where $\underline{y}$ is a vector of phase fractions y_i present at a mesodomain.

2.2 Balance Laws for TMM Process

The mathematical model of TMM process consist of two principles expressing thermal and mechanical equilibrium, i.e. the balance of internal energy and the balance of momentum which are supplemented by phase evolution laws. These principles have been derived to account for the coupling of thermal, mechanical and metallurgical effects for a thermo-inelastic body with solid phase transformations. The equilibrium equation for solid is given by the following equations:

$$(\tilde{S}_{KL} x_{i,L})_{,K} - \rho_0 \, b_i = 0 \tag{6}$$

for particle $\mathbf{X} \in V$, and

$$\tilde{S}_{KL} x_{i,L} N_K = T_i \tag{7}$$

for the particle $\mathbf{X} \in \partial V$, where b_i is the body force, T_i is the nominal stress vector. Assuming the actual coordinate system $\{x_i\}$ which is collinear with the reference coordinate system $\{X_I\}$ these equations can be rewritten in the forms

$$(\tilde{S}_{KI} + \tilde{S}_{KL} u_{I,L})_{,K} - \rho_0 \, b_I = 0 \tag{8}$$

$$(\tilde{S}_{KI} + \tilde{S}_{KL} u_{I,L}) N_K = T_I \tag{9}$$

The local balance of internal energy - the first law of thermodynamics for non-rigid conductor is expressed by two following equations that are appropriate for volume and surface distributions of internal and kinetic energies [8], [19]. The first equation, valid for particles $\mathbf{X} \in V$, can be written as the following:

$$\rho\dot{e} + div\mathbf{q} - \tilde{\mathbf{S}} : \dot{\tilde{\mathbf{E}}} - \rho\mathcal{R} - \sum_{\mathcal{J}} \mathcal{F}_{\theta}^{\mathcal{J}} = 0, \tag{10}$$

where e is the "heat energy" density per unit mass, its rate is given by $\dot{e} = \frac{\partial e}{\partial t}$, the vector of heat flux transferred through the particle $\mathbf{X} \in V$ is called $\mathbf{q}$, concentrated heat fluxes are $\sum_{\mathcal{J}} \mathcal{F}_{\theta}^{\mathcal{J}}$, and $\mathcal{R}$ is the radiation of entropy per unit mass. The rate of mechanical energy is $\tilde{\mathbf{S}} : \dot{\tilde{\mathbf{E}}}$.

Assuming that the region Γ^{pt} where phase transformations proceed can be idealized by the singular surface $\partial\Gamma^{pt}$, the second equation, appropriate for particles $\mathbf{X} \in \Gamma^{pt}$, can be written in the form

$$\dot{e}^{su} - 2v_N^{pt}\mathcal{C}_{me}\, e^{su} = e^{su^*} + \left|\left[\rho v^{pt}\left(\frac{1}{2}\mathbf{V}\cdot\mathbf{V} + e\right) + \mathbf{V}\cdot\tilde{\mathbf{S}}\cdot\mathbf{N}^{\Gamma} - \mathbf{q}\cdot\mathbf{N}^{\Gamma} \right]\right| \tag{11}$$

where e^{su} is the surface concentration of the specific energy, e^{su^*} is the surface source of energy, v^{pt} and v_N^{pt} is the speed and normal speed of $\partial\Gamma^{pt}$, $\mathcal{C}_{me}$ is the mean curvature of the surface, $\mathbf{V}$ is the velocity of particle $\mathbf{X}$, $\mathbf{N}^{\Gamma}$ is the singular surface normal. The double square brackets |[...]|, defined in [8] and [19], denote the difference of the bracketed quantity on the two sides of the surface $\partial\Gamma^{pt}$.

The indical forms of Eqs.(10) and (11) are

$$\rho\dot{e} + q_{I,I} - \tilde{S}_{IJ}\,\dot{\tilde{E}}_{IJ} - \rho\mathcal{R} - \sum_{\mathcal{J}} \mathcal{F}_{\theta}^{\mathcal{J}} = 0, \tag{12}$$

for particle $\mathbf{X} \in V$,

$$\dot{e}^{su} - 2v_N^{pt}\mathcal{C}_{me}\, e^{su} = \left|\left[\rho v^{pt}\left(\frac{1}{2}\, V_K\, V_K + e\right) + V_K\,\tilde{S}_{KL}\, N_K^{\Gamma} - q_K\, N_K^{\Gamma} \right]\right| + e^{su^*}; \tag{13}$$

for particle $\mathbf{X} \in \partial\Gamma^{pt}$.

Considering derivations shown in [13] and [19], the following substitutions can be done

$$\begin{aligned} \dot{e} &= C_v\dot{\theta} \\ \mathbf{q} &= \mathbf{k}\cdot\nabla\theta \\ div\mathbf{q} &= \nabla\cdot\mathbf{q} \\ \nabla\{\mathbf{k}\cdot\nabla\theta\} &= \{\mathbf{k}\cdot\nabla\}\nabla\theta + \{\nabla\theta\cdot\nabla\}\mathbf{k} + \\ & \quad \nabla\theta\times\{\nabla\times\mathbf{k}\} \end{aligned} \tag{14}$$

where C_v is the specific heat per unit mass referred to constant volume, $\nabla \equiv \mathbf{n}^J \frac{\partial}{\partial X^J}$ is the vector differential operator **nabla** whose "components" $\frac{\partial}{\partial X^J}$ transform like covariant vector components, $\mathbf{n}^J$ is the J-th base vector. The diagonal tensor of thermal conductivity $\mathbf{k}$ is defined by

$$k = \begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{bmatrix} \tag{15}$$

This matrix is usually considered to be isotropic, although anisotropic coefficients of conductivity are used to simulate droplet penetration [11]. Such relations are given for k_{22} and k_{33} in the forms

$$\begin{aligned} k_{22} &= k_{me}\left(1 + 3\exp\left(\frac{-r^2}{2\delta_r^2}\right)\right) \\ k_{33} &= k_{me}\left(1 + 10\exp\left(\frac{-r^2}{2\delta_r^2}\right)\right) \\ k_{22} &= k_y;\ k_{33} = k_z \end{aligned} \tag{16}$$

where k_{me} is the mean conductivity, r is the horizontal distance from the weld center, and δ_r is the standard deviation of heat distribution measured in mm. The z direction is vertically perpendicular to the weld and the y direction is parallel to arc motion.

The expression for $\nabla\{\mathbf{k}\cdot\nabla\theta\}$ in Eq.(14) can be simplified assuming thermal homogeneity of inelastic conductor, that leads to the assumption: $k_{IJ}(\mathbf{X}) = \text{const}, \forall\mathbf{X} \in V$. Hence it can be expressed by

$$\nabla\{\mathbf{k}\cdot\nabla\theta\} = \{\mathbf{k}\cdot\nabla\}\nabla\theta \equiv \mathbf{k}\cdot\nabla^2\theta \tag{17}$$

with the Laplacian operator ∇^2. This can be rewritten in the indical form as

$$q_{I,I} = k_{IJ}\theta_{,JI}. \tag{18}$$

The balance of internal energy for inelastic conductor can be written in the form of "the improved heat equation" substituting Eq.(18) to Eq.(12), and introducing concentrated heat fluxes modelling either separate one-point chemical reactions or laser-beam welding. Such a "heat equation" can be expressed by

$$c\dot{\theta} + k_{IJ}\theta_{,JI} = f_{\theta}^{M} + \sum_{\mathcal{J}} \mathcal{F}_{\theta}^{\mathcal{J}} + \rho\,\mathcal{R}, \tag{19}$$

where the rate of mechanical energy is $f_{\theta}^{M} = \tilde{S}_{KL}\dot{\tilde{E}}_{KL}$, specific heat is $c = \rho C_v$.

Balance laws for momentum and internal energy can be expressed in the functional forms and then approximated by the Galerkin type Finite Element Method. A formulation of the functional forms of the balance laws consist of the following steps [7], [13]:

- Characterize two classes of functions: the trial solutions $\mathcal{U}$ and the weighting functions $\mathcal{V}$ (or variations), which are defined by

$$\mathcal{U} = \{u, \theta \mid u, \theta \in H^1\} \tag{20}$$

where u and θ fulfills boundary conditions for the thermo-mechanical problem,

$$\mathcal{V} = \{v, \vartheta\} \mid \ v, \vartheta \in H^1\} \tag{21}$$

where u, ϑ are equal zero at the boundary ∂V, and H^1 is the Hilbert space.

- Express the balance laws Eqs.(8), (9), (14), (19), as differential operators defined by

$$\Phi_V(\mathbf{u}) = (\tilde{S}_{KI} + \tilde{S}_{KL} u_{I,L})_{,K} - \rho_0 \, b_I = 0 \; ; \tag{22}$$

$$\Phi_{\partial V}(\mathbf{u}) = (\tilde{S}_{KI} + \tilde{S}_{KL} u_{I,L}) N_K - T_I = 0 \; ; \tag{23}$$

$$\begin{aligned} \Psi_V(\theta) &= c\dot{\theta} + k_{IJ}\theta_{,JI} - f_\theta^M \\ &- \sum_{\mathcal{J}} \mathcal{F}_\theta^{\mathcal{J}} - \rho\, \mathcal{R} = 0 \; ; \end{aligned} \tag{24}$$

$$\begin{aligned} \Psi_{\partial V}(\theta) &= \dot{e}^{su} - 2v_N^{pt} \mathcal{C}_{me} \, e^{su} - e^{su^*} \\ &- \Big|\Big[\rho v^{pt} \left(1/2 \; V_K \; V_K + e\right) \\ &+ V_K \, \tilde{S}_{KL} \, N_K^\Gamma - q_K \, N_K^\Gamma \Big]\Big| . \end{aligned} \tag{25}$$

- Take scalar products of these operators and weighting functions v and ϑ, correspondingly,

$$\int_{V_0} \left(\tilde{S}_{KI} + \tilde{S}_{KL} u_{I,L} \right)_{,K} v_I dV - \int_{V_0} b_I v_I dV = 0; \tag{26}$$

$$\int_{\partial V_0} (\tilde{S}_{KI} + \tilde{S}_{KL} u_{I,L}) N_K v_I \; d\mathcal{P} - \int_{\partial V_0} T_I v_I \; d\mathcal{P} = 0; \tag{27}$$

$$\int_{V_0} \left(c\dot{\theta} + k_{IJ}\theta_{,JI} \right) \vartheta dV - \int_{V_0} f_\theta^M \; \vartheta dV - \sum_{\mathcal{J}} \mathcal{F}_\theta^{\mathcal{J}} \vartheta \mid_{\mathcal{J}} - \int_{V_0} \rho \mathcal{R} \; \vartheta dV = 0; \tag{28}$$

$$\begin{aligned} &\int_{\partial \Gamma^{pt}} \left(\dot{e}^{su} - 2v_N^{pt} \mathcal{C}_{me} \, e^{su} - e^{su^*} \right) \vartheta \; d\mathcal{P} \\ &- \int_{\partial \Gamma^{pt}} \Big|\Big[\rho \, v^{pt} \; e + q_K \; N_K^\Gamma \Big]\Big| \vartheta \; d\mathcal{P} \\ &- \int_{\partial \Gamma^{pt}} \Big|\Big[1/2 \; \rho \; v \; V_K \; V_K \\ &+ V_K \; \tilde{S}_{KL} \; N_K^\Gamma \Big]\Big| \vartheta \; d\mathcal{P} = 0. \end{aligned} \tag{29}$$

- Write the system of two variational equations equivalent to the system of four equations after amalgamation of pairs of equations: Eq.(26) with Eq.(27), and Eq.(28) with Eq.(29), and balancing surface projections:

$$\left(\tilde{S}_{KI} + \tilde{S}_{KL} u_{I,L} \right) v_I \; \text{ on surface } \partial V_0,$$

$$\frac{1}{2} \left(\rho v^{pt} V_K V_K + V_K \; \tilde{S}_{KL} \; N_K^\Gamma \right) \vartheta \; \text{ on } \partial \Gamma^{pt}.$$

Such equations have the following forms:

$$\int_{V_0} \left(\tilde{S}_{KI} + \tilde{S}_{KL} u_{I,L} \right)_{,K} v_I dV - \int_{V_0} b_I v_I dV - \int_{\partial V_0} T_I v_I \; d\mathcal{P} = 0; \tag{30}$$

$$\begin{aligned} &\int_{V_0} \left(c\dot{\theta} + k_{IJ}\theta_{,JI} \right) \vartheta dV - \int_{V_0} f_\theta^M \; \vartheta dV \\ &- \int_{\partial \Gamma^{pt}} f_\theta^{su} \; \vartheta d\mathcal{P} - \int_{\partial \Gamma^{pt}} f_\theta^\Gamma \; \vartheta d\mathcal{P} \\ &- \sum_{\mathcal{J}} \mathcal{F}_\theta^{\mathcal{J}} \vartheta \mid_{\mathcal{J}} - \int_{V_0} f_\theta^r \; \vartheta d\mathcal{P} = 0, \end{aligned} \tag{31}$$

where

$$\begin{aligned} f_\theta^r &\equiv \rho \, \mathcal{R}; \\ f_\theta^{su} &\equiv \dot{e}^{su} - 2v_N^{pt} \mathcal{C}_{me} \, e^{su} - e^{su^*}; \\ f_\theta^\Gamma &\equiv \Big|\Big[\rho \; v^{pt} \; e + q_K \; N_K^\Gamma \Big]\Big| . \end{aligned}$$

- Use the Green formula to decompose the first integral of Eq.(30)

$$\begin{aligned} &\int_{V_0} \left(\tilde{S}_{KI} + \tilde{S}_{KL} u_{I,L} \right)_{,K} v_I dV \\ &= \int_{V_0} \left(\tilde{S}_{KI,K} + \tilde{S}_{KL,K} u_{I,L} \right) v_I dV \\ &+ \int_{\partial V_0} \tilde{S}_{KL} u_{I,L} v_I \; d\mathcal{P} \\ &- \int_{V_0} \tilde{S}_{KL} u_{I,L} v_{I,K} dV \end{aligned} \tag{32}$$

where the second integral of R.H.S. vanishes because of the boundary conditions for the weighting function $v \in \mathcal{V}$.

- Use the Green formula to decompose the integral with the divergence of temperature in the heat equation

$$\int_{V_0} k_{IJ}\theta_{,JI} \vartheta dV = \int_{\partial V_0} k_{IJ}\theta_{,I} \, \vartheta d\mathcal{P} - \int_{V_0} k_{IJ} \, \theta_{,I} \, \vartheta_{,J} \, dV \tag{33}$$

where the integral $\int_{\partial V_0} k_{IJ}\theta_{,I} \, \vartheta d\mathcal{P}$ includes in- and out-fluxes due to conduction, convection, and radiation through the external surface of welded body.

- Combination of the above decompositions with Eq.(30) and Eq.(31) gives

$$\begin{aligned} &\int_{V_0} \tilde{S}_{KL} u_{I,L} v_{I,K} dV - \\ &\int_{V_0} \left(\tilde{S}_{KI,K} + \tilde{S}_{KL,K} u_{I,L} \right) v_I dV \\ &+ \int_{V_0} b_I v_I dV + \int_{\partial V_0} T_I v_I \; d\mathcal{P} = 0 \end{aligned} \tag{34}$$

$$\int_{V_0} k_{IJ}\,\theta_{,I}\,\vartheta_{,J}\,dV - \int_{V_0} c\dot{\theta}\,\vartheta dV + \int_{V_0} f_\theta^M\,\vartheta dV - \int_{\partial V_0} f_\theta^{\partial V}\,\vartheta d\mathcal{P} + \int_{\partial\Gamma^{pt}} f_\theta^{su}\,\vartheta d\mathcal{P} + \int_{\partial\Gamma^{pt}} f_\theta^{\Gamma}\,\vartheta d\mathcal{P} + \sum_{\mathcal{J}} \mathcal{F}_\theta^{\mathcal{J}}\vartheta\mid_{\mathcal{J}} + \int_{V_0} f_\theta^r\,\vartheta d\mathcal{P} = 0 \tag{35}$$

where

$$\int_{\partial V_0} f_\theta^{\partial V}\,\vartheta d\mathcal{P} = \int_{\partial V_0} k_{IJ}\theta_{,I}\,\vartheta d\mathcal{P} \tag{36}$$

Stationary conditions for functionals Eq.(34) and Eq.(35) are the following variational equations:

$$\int_{V_0} \tilde{S}_{KL}u_{I,L}\,\delta v_{I,K}dV - \int_{V_0}\left(\tilde{S}_{KI,K} + \tilde{S}_{KL,K}u_{I,L}\right)\delta v_I dV + \int_{V_0} b_I\,\delta v_I dV + \int_{\partial V_0} T_I\,\delta v_I\,d\mathcal{P} = 0 \tag{37}$$

$$\int_{V_0} k_{IJ}\,\theta_{,I}\,\delta\vartheta_{,J}\,dV - \int_{V_0} c\dot{\theta}\,\delta\vartheta dV + \int_{V_0} f_\theta^M\,\delta\vartheta dV - \int_{\partial V_0} f_\theta^{\partial V}\,\delta\vartheta d\mathcal{P} + \int_{\partial\Gamma^{pt}} f_\theta^{su}\,\delta\vartheta d\mathcal{P} + \int_{\partial\Gamma^{pt}} f_\theta^{\Gamma}\,\delta\vartheta d\mathcal{P} + \sum_{\mathcal{J}} \mathcal{F}_\theta^{\mathcal{J}}\delta\vartheta\mid_{\mathcal{J}} + \int_{V_0} f_\theta^r\,\delta\vartheta dV = 0 \tag{38}$$

which are obtained by using the Gateaux derivatives appropriate for discontinuous temperature field ϑ, the term $\int_{\partial\Gamma^{pt}} f_\theta^\Gamma\,\vartheta d\mathcal{P}$, and continuous displacement field v. The equation Eq.(37) is called the equation of virtual work. Solutions of these variational equations, v and ϑ, are called the weak, or generalized, solutions.

3. Stress-Strain Constitutive Equations and Tangent Moduli

Deformations of microregion V^{mic} of an alloy with multiphase internal structure occur due to phase transformations driven by variations of temperature and stress, external thermal and mechanical loadings and internal energy sources. A microregion deformation is separated into reversible and permanent parts, and therefore appropriate elastic, thermal and plastic components of Green-Lagrange finite strain rate tensor are counted in the total strain rate evaluation. The total strain rate $\dot{\mathbf{L}}$ can be divided into five terms

$$\dot{\mathbf{L}} = \dot{\mathbf{L}}^{el} + \dot{\mathbf{L}}^{th} + \dot{\mathbf{L}}^{tr} + \dot{\mathbf{E}}^{pl} + \dot{\mathbf{E}}^{trip} \tag{39}$$

with $\dot{\mathbf{L}}^{el}$ elastic strain rate, $\dot{\mathbf{L}}^{th}$ thermal strain rate, $\dot{\mathbf{L}}^{tr}$ transformation strain rate, $\dot{\mathbf{E}}^{pl}$ plastic strain rate, and $\dot{\mathbf{E}}^{trip}$ plastic strain rate induced by phase transformation marked with ^{trip} which is the abbreviation issued from the TRansformation Induced Plasticity. The strain rate $\dot{\mathbf{L}}$ can be also split into a spherical and deviatoric part

$$\dot{\mathbf{L}} = \frac{1}{3}\,\mathrm{tr}\dot{\mathbf{L}}\cdot\mathbf{1} + \dot{\mathbf{E}} \tag{40}$$

which are defined in terms of the second-order tensor components

$$\frac{1}{3}\,\mathrm{tr}\dot{\mathbf{L}} = \frac{1}{3}\dot{L}_{KK} = \frac{1}{3}\left(\dot{L}_{KK}^{el} + \dot{L}_{KK}^{th} + \dot{L}_{KK}^{tr}\right), \tag{41}$$

$$\dot{E}_{IJ} = \dot{E}_{IJ} - \frac{1}{3}\delta_{IJ}tr\dot{\mathbf{L}} = \dot{E}_{IJ}^{pl} + \dot{E}_{IJ}^{trip} + \dot{E}_{IJ}^{el}. \tag{42}$$

3.1 Elastic Strain and Thermal Dilatation

The spherical part of elastic strain rate $\mathrm{tr}\dot{\mathbf{L}}^{el}$ and the deviator of elastic strain rate $\dot{\mathbf{E}}^{el}$ are related to stress rate $\dot{\mathbf{T}}$ by Hooke's law

$$\mathrm{tr}\dot{\mathbf{T}} = \kappa\left(\mathrm{tr}\dot{\mathbf{L}} - \dot{L}_{KK}^{th} - \dot{L}_{KK}^{tr}\right) + \frac{\dot{\kappa}}{\kappa}\,\mathrm{tr}\mathbf{T}, \tag{43}$$

$$\dot{\mathbf{S}}_{IJ} = 2\mu\left(\dot{E}_{IJ} - \dot{E}_{IJ}^{pl} - \dot{E}_{IJ}^{trip}\right) + \frac{\dot{\mu}}{\mu}\mathbf{S}_{IJ}, \tag{44}$$

with the bulk modulus $\langle\kappa\rangle$ and the shear modulus $\langle\mu\rangle$ defined by

$$\langle\kappa\rangle = \frac{\langle E(\theta)\rangle}{1-2\langle\nu(\theta)\rangle};\quad \langle\mu\rangle = \frac{\langle E(\theta)\rangle}{2\left(1+\langle\nu(\theta)\rangle\right)}, \tag{45}$$

where the Young's modulus $\langle E\rangle$ and the Poisson's ratio $\langle\nu\rangle$ are averaged accordingly to the linear mixture law

$$\langle E(\theta)\rangle = E_i(\theta)y_i;\quad \langle\nu(\theta)\rangle = \nu_i(\theta)y_i. \tag{46}$$

The spherical part of thermal strain rate $\mathrm{tr}\dot{\mathbf{L}}^{th} = \dot{L}_{KK}^{th}$ represents the thermal expansion of different phases and at inhomogeneous microregion is defined by

$$\mathrm{tr}\dot{\mathbf{L}}^{th} = \frac{d}{dt}\left(y_i\int_0^{\theta(t)} {}_i\alpha_{JK}^{dil}(\vartheta)\delta_{KJ}d\vartheta\right) = \dot{y}_i\int_0^{\theta(t)} {}_i\alpha_{JK}^{dil}(\vartheta)\delta_{KJ}d\vartheta + \frac{1}{3}\,{}_i\alpha_{KK}^{dil}\,y_i\,\dot{\theta} \tag{47}$$

with the diagonal tensor ${}_i\alpha_{JK}^{dil}(\theta)$ representing the temperature dependent thermal expansion coefficients of phase constituent i.

The transformation strain rate $\dot{\mathbf{E}}^{tr}$ is associated with the expansion generated by the change of parent phase density ie. austenite density ρ_{aus} into the daughter phase density ρ_i, $i = 2, ..., 6$. The spherical part of this strain rate is evaluated by

$$\frac{1}{3}\,\mathrm{tr}\dot{\mathbf{L}}^{tr} = \frac{1}{3}\alpha_i^{tra}\dot{y}_i \tag{48}$$

with the transformation expansion coefficient α_i^{tra} defined by

$$\alpha_i^{tra} = \frac{\rho_{aus}^{0^\circ C} - \rho_i}{\rho_{aus}^{0^\circ C}} \tag{49}$$

where austenite density ρ_{aus} is taken at temperature $0^\circ C$.

3.2 Inelastic Strain Decomposition

3.2.1 Classical Plasticity

The plastic strain rates $\dot{\mathbf{E}}^{pl}$ are evaluated using the Huber-Von Mises yield condition and the associated flow rule. The yield surface with the isotropic and kinematic hardening effects is defined by

$$f = \phi(\Sigma_{KL}) - \kappa(W^{pl}, \theta, y_i); \tag{50}$$

where Σ_{KL} is the effective stress deviator defined later in this chapter, and the plastic work is given by

$$W^{pl} = \int S_{IJ}\ \dot{E}_{IJ}^{pl}\ dt, \tag{51}$$

with the hardening function κ. As the function $f(S_{IJ})$ is a potential for strain and a plastic strain rate is normal to the yield surface, $f(S_{IJ}) = 0$, the following flow law can be written:

$$\dot{E}_{IJ}^{pl} = \Lambda_{IJ} = \dot{\Lambda}\frac{\partial f}{\partial S_{IJ}}, \tag{52}$$

That can be also expressed in incremental form

$$\Delta E_{IJ}^{pl} = \bar{\Lambda}\frac{\partial f}{\partial S_{IJ}}, \tag{53}$$

where $\bar{\Lambda}$ is the plastic function related to stress, strain, strain rate, temperature, as well as phase fractions, and it is, as yet, undetermined proportionality factor or plastic multiplier. The plastic strain increment fulfills the following conditions for unloading of generalized particle:

$$\Delta E_{IJ}^{pl} = 0 \begin{cases} f(S_{IJ}) < 0 \\ f(S_{IJ}) = 0 \quad \text{and} \quad \Delta E_{IJ} : S_{IJ} < 0 \end{cases} \tag{54}$$

3.2.2 Tangent Moduli and the Solution Algorithm for Determining the Plastic Strain Rate Multiplier, Λ

The algorithmic or consistent tangent moduli is used in forming the finite element stiffness matrices $K_{uu}, K_{u\theta}, K_{\theta u}$ to ensure quadratic convergence of the global Newton-Raphson solution scheme. These matrices arise from algorithm for the time integration of the plastic strain rate.

A yield criterion for assessment of plastic flow is expressed by

$$f(\mathbf{S}, H_\alpha, K_\alpha) = ||\mathbf{\Sigma}|| - \sqrt{\frac{2}{3}}K_\alpha = 0 \tag{55}$$

where two hardening effects are represented by isotropic, K_α, and kinematic, H_α, hardening parameters. These parameters are related to equivalent plastic strain $\bar{E}^{pl} = \sqrt{\frac{2}{3}}||\mathbf{E}^{pl}||$, equivalent strain rate $\dot{E}^{eq} = \frac{1}{\Delta t}(\frac{2}{3}\Delta\mathbf{E} : \Delta\mathbf{E})^{\frac{1}{2}}$, and temperature θ, that symbolically can be written as $K_\alpha = K_\alpha(\bar{E}^{pl}, \dot{E}^{eq}, \theta)$ and $H_\alpha = H_\alpha(\bar{E}^{pl}, \dot{E}^{eq}, \theta)$.

The effective stress defined by

$$\mathbf{\Sigma} = \mathbf{S} - \mathbf{Z} \tag{56}$$

appears in the yield criterion rather than the usual deviatoric stress $\mathbf{S}$. The back stress $\mathbf{Z}$ is determined incrementally form the expression

$$\mathbf{Z}^{n+1} = \mathbf{Z}^n + \sqrt{\frac{2}{3}}\Delta H_\alpha \mathbf{n} \tag{57}$$

A predictor - corrector method is used to determine the unknown value of the plastic strain increment $\bar{\Lambda} = \Delta t\dot{\Lambda}$. This increment is determined at time step $n+1$ by using the backward Euler implicit method. Assuming that current increment is purely elastic, the starting values of the variables are set up and hence $\dot{\Lambda} = 0$. These starting values are known as the elastic predicted ones:

$$\mathbf{S}^* = \mathbf{S}_n + 2\langle\mu\rangle\Delta\mathbf{E}^x \quad , \quad \mathbf{\Sigma}^* = \mathbf{S}^* - \mathbf{Z}_n \tag{58}$$

where the deviatoric part of the strain increment is used without accounting for the thermal and transformation plastic strains, and given by

$$\Delta\mathbf{E}^x = \mathbf{I}_{dev} : \left[\Delta\mathbf{L} - \langle\alpha^{thm}\rangle\mathbf{1}\Delta\theta - \frac{1}{3}\,\mathrm{tr}\Delta\mathbf{L}^{tp}\mathbf{1}\right] \tag{59}$$

The fourth order tensor $\hat{\mathbf{I}}_{dev}$ is an operator converting a second order tensor to its deviator and is defined by $\hat{\mathbf{I}}_{dev} = \hat{\mathbf{I}} - \frac{1}{3}\mathbf{1}\otimes\mathbf{1}$, where $\mathbf{I}$ and $\mathbf{1}$ are the fourth and second order unit tensors, correspondingly.

The direction of plastic flow for an associate flow rule (J_2) is in the direction of applied stress which may be determined assuming a purely elastic increment.

The direction $\mathbf{n}$ normal to the yield surface is given by:

$$\mathbf{n} = \frac{\mathbf{\Sigma}^*}{||\mathbf{\Sigma}^*||}. \tag{60}$$

The formula for the effective stress calculation can be determined from Eq.(56) and the additive decomposition of strain rates expressed by Eq.(39), and can be written as

$$\mathbf{\Sigma} = \mathbf{\Sigma}^* - 2\langle\mu\rangle\Delta t\left[\dot{\mathbf{E}}^{pl} + \dot{\mathbf{E}}^{trip}\right] - \sqrt{\frac{2}{3}}\Delta H_\alpha \mathbf{n} \tag{61}$$

Substituting this equation to the yield criterion leads to

$$\begin{aligned} f(\bar{\Lambda}) \quad & \equiv ||\mathbf{\Sigma}|| - \sqrt{\frac{2}{3}}K_\alpha \leq 0 \\ \Leftrightarrow \quad & ||\mathbf{\Sigma}^* - 2\langle\mu\rangle\Delta t\left[\dot{\mathbf{E}}^{pl} + \dot{\mathbf{E}}^{trip}\right] - \\ & \sqrt{\frac{2}{3}}\Delta H_\alpha\mathbf{n}|| - \sqrt{\frac{2}{3}}K_\alpha \leq 0 \\ \Leftrightarrow \quad & \Big\|\mathbf{\Sigma}^* - 2\langle\mu\rangle\bar{\Lambda}\mathbf{n} - 2\langle\mu\rangle\Delta t\dot{\mathbf{E}}^{trip} \\ & -\sqrt{\frac{2}{3}}\Delta H_\alpha\mathbf{n}\Big\| - \sqrt{\frac{2}{3}}K_\alpha \leq 0. \end{aligned} \tag{62}$$

The inequality condition is satisfied when the increment of strain is purely elastic, and the equality is appropriate for the case of plastic strain increment.

The plastic corrector algorithm is the following:

1) calculate the derivative:

$$\begin{aligned} \frac{\partial f(\bar{\Lambda})}{\partial\bar{\Lambda}} &= \frac{2}{3}K'_\alpha - \gamma\frac{\mathbf{\Sigma}}{||\mathbf{\Sigma}||} : \mathbf{n}\left[2\langle\mu\rangle + \frac{2}{3}H'_\alpha\right] \\ &= \frac{2}{3}K'_\alpha - \gamma\left[2\langle\mu\rangle + \frac{2}{3}H'_\alpha\right] \end{aligned} \tag{63}$$

where

$$\gamma = \frac{1}{1 + 2\langle\mu\rangle\Delta t E_\alpha^{trip}} \tag{64}$$

with the transformation induced plastic strain rate given by

$$\dot{\mathbf{E}}^{trip} = E_\alpha^{trip}\mathbf{\Sigma}$$

The functional form of this relation will be derived later and shown as Eq.(82).

2) update $\bar{\Lambda}$ applying the Newton-Raphson scheme

$$\bar{\Lambda}^{(k+1)} = \bar{\Lambda}^{(k)} - f(\bar{\Lambda})\left[\frac{\partial f(\bar{\Lambda})}{\partial\bar{\Lambda}}\right]^{-1} \tag{65}$$

3) update the plastic strain using the current value of the plastic strain increment

$$\begin{aligned} \bar{E}^{pl}_{n+1} &= \bar{E}^{pl}_n + \int_t \sqrt{\frac{2}{3}}||\dot{\mathbf{E}}^{pl}||dt \\ &= \bar{E}^{pl}_n + \sqrt{\frac{2}{3}}\bar{\Lambda} \end{aligned} \tag{66}$$

4) update hardening functions: ΔH_α , K_α for the $k+1$ iteration of $\bar{\Lambda}$,

5) check the relation: $f(\bar{\Lambda}) <$ TOL, and terminate the procedure when this condition is fulfilled, otherwise repeat the above sequence of evaluations again.

Stress is calculated either by

$$\mathbf{S}^{(k+1)}_{n+1} = \mathbf{Z}^{(k+1)}_{n+1} + \sqrt{\frac{2}{3}}K_\alpha\,\mathbf{n}, \tag{67}$$

when the strain increment is plastic or $\mathbf{S}_{n+1} = \mathbf{S}^*$ when the strain increment is elastic.

The full stress tensor is calculated by adding the deviatoric stress and the spherical part of stress, ie.

$$\mathbf{T}_{n+1} = \mathbf{S}_{n+1} + \frac{1}{3}\,\mathrm{tr}\mathbf{T}^*\,\mathbf{1}, \tag{68}$$

where $\mathbf{T}^*$ is the stress predicted for elastic reaction of an alloy.

The tangent modulus $\frac{\partial\mathbf{T}}{\partial\mathbf{L}}$ at the particular time step $n+1$ is defined by

$$\begin{aligned} \frac{\partial\mathbf{T}}{\partial\mathbf{L}} &= \frac{\partial}{\partial\mathbf{L}}\Big\{\langle\kappa\rangle\left[\mathrm{tr}\Delta\mathbf{L} - \mathrm{tr}\Delta\mathbf{L}^{tp} - \langle\alpha^{thm}\rangle\Delta\theta\right]\mathbf{1} \\ &\quad +\mathbf{Z} + \sqrt{\frac{2}{3}}K_\alpha\mathbf{n} + 2\langle\mu\rangle\Delta\mathbf{E}^{trip}\Big\}\Big|_{n+1} \\ &= \langle\kappa\rangle\mathbf{1}\otimes\mathbf{1} + \frac{\partial\mathbf{Z}}{\partial\mathbf{L}}\Big|_{n+1} + \sqrt{\frac{2}{3}}\frac{\partial K_\alpha}{\partial\mathbf{L}}\Big|_{n+1}\otimes\mathbf{n} \\ &\quad +2\langle\mu\rangle\frac{\partial\Delta\mathbf{E}^{trip}}{\partial\mathbf{L}}\Big|_{n+1} \end{aligned} \tag{69}$$

where derivative of the back stress expressed in terms of hardening parameters is

$$\begin{aligned} \frac{\partial\mathbf{Z}}{\partial\mathbf{L}}\Big|_{n+1} &= \mathbf{n}\otimes\sqrt{\frac{2}{3}}\frac{\partial H_\alpha}{\partial\mathbf{L}}\Big|_{n+1} \\ &= \mathbf{n}\otimes\left[\sqrt{\frac{2}{3}}\frac{\partial H_\alpha}{\partial\bar{E}^{pl}}\frac{\partial\bar{E}^{pl}}{\partial\mathbf{E}} : \frac{\partial\mathbf{E}}{\partial\mathbf{L}}\right. \\ &\quad \left.+\sqrt{\frac{2}{3}}\frac{\partial H_\alpha}{\partial\dot{E}^{eq}}\frac{\partial\dot{E}^{eq}}{\partial\mathbf{E}} : \frac{\partial\mathbf{E}}{\partial\mathbf{L}}\right]_{n+1} \\ &= \mathbf{n}\otimes\left[\sqrt{\frac{2}{3}}\frac{\partial H_\alpha}{\partial\bar{E}^{pl}}\hat{\mathbf{I}}_{dev} : \frac{\partial\bar{E}^{pl}}{\partial\bar{\Lambda}}\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}} + \right. \\ &\quad \sqrt{\frac{2}{3}}H^r_\alpha\frac{1}{2\Delta t}\left(\frac{3}{2}\Delta\mathbf{E} : \Delta\mathbf{E}\right)^{-\frac{1}{2}} \end{aligned}$$

$$\begin{aligned}&2\mathbf{E}:\left.\frac{\partial \mathbf{E}}{\partial \mathbf{L}}\right]_{n+1}\\ &= \mathbf{n}\otimes\left[\frac{2}{3}H'_\alpha \hat{\mathbf{I}}_{dev}:\frac{\partial\bar{\Lambda}}{\partial \mathbf{E}}\right.\\ &\left.+\sqrt{\frac{2}{3}}H^r_\alpha\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}\right]_{n+1}\end{aligned} \tag{70}$$

and the derivative of the isotropic hardening function is

$$\begin{aligned}\mathbf{n}\otimes\sqrt{\frac{2}{3}}\left.\frac{\partial K_\alpha}{\partial \mathbf{L}}\right|_{n+1} &= \mathbf{n}\otimes\left[\frac{2}{3}K'_\alpha\hat{\mathbf{I}}_{dev}:\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}\right.\\ &\left.+\sqrt{\frac{2}{3}}K^r_\alpha\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}\right]_{n+1}.\end{aligned} \tag{71}$$

The derivative of the transformation induced plastic strain increment in Eq.(69) can be expressed by

$$\begin{aligned}&2\langle\mu\rangle\left.\frac{\partial\Delta\mathbf{E}^{trip}}{\partial\mathbf{L}}\right|_{n+1}\\ &= 2\langle\mu\rangle\Delta t\frac{\partial}{\partial\mathbf{L}}\left[E^{trip}_\alpha\boldsymbol{\Sigma}\right]_{n+1}\\ &= 2\langle\mu\rangle\Delta t E^{trip}_\alpha\frac{\partial}{\partial\mathbf{L}}\left[\gamma(\boldsymbol{\Sigma}^*-2\langle\mu\rangle\bar{\Lambda}\mathbf{n}\right.\\ &\left.-\sqrt{\frac{2}{3}}\Delta H_\alpha\mathbf{n})\right]_{n+1}\\ &= \bar{\gamma}\left[2\langle\mu\rangle\hat{\mathbf{I}}_{dev}-2\langle\mu\rangle\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}:\hat{\mathbf{I}}_{dev}\otimes\mathbf{n}\right.\\ &-\hat{\mathbf{I}}_{dev}:\left\{\frac{2}{3}H'_\alpha\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}+\sqrt{\frac{2}{3}}H^r_\alpha\frac{1}{\Delta t}\right.\\ &\left.\left.\frac{\Delta\mathbf{E}}{\Delta E^{eq}}\right\}\otimes\mathbf{n}\right]_{n+1}\\ &= \bar{\gamma}\hat{\mathbf{I}}_{dev}:\left[2\langle\mu\rangle\hat{\mathbf{I}}-2\langle\mu\rangle\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}\otimes\mathbf{n}\right.\\ &-\left.\left\{\frac{2}{3}H'_\alpha\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}+\sqrt{\frac{2}{3}}H^r_\alpha\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}\right\}\otimes\mathbf{n}\right]_{n+1},\end{aligned} \tag{72}$$

where

$$\bar{\gamma}=\gamma 2\langle\mu\rangle\Delta E^{trip}_\alpha \tag{73}$$

The derivative $\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}$ occurring in the above expression is still unknown and it can be obtained by the implicit differentiation technique applied to the yield condition when assuming that plastic yielding occurs within the increment Δt and $\Lambda\neq 0$, so that

$$\begin{aligned}&\left\|\gamma(\|\boldsymbol{\Sigma}^*\|\mathbf{n}-2\langle\mu\rangle\bar{\Lambda}\mathbf{n})\right.\\ &\left.-\sqrt{\frac{2}{3}}\Delta H_\alpha\mathbf{n}-\sqrt{\frac{2}{3}}K_\alpha\mathbf{n}\right\| =\\ &\left[\gamma\left\{\|\boldsymbol{\Sigma}^*\|-2\langle\mu\rangle\bar{\Lambda}-\sqrt{\frac{2}{3}}\Delta H_\alpha\right\}\right.\\ &\left.-\sqrt{\frac{2}{3}}K_\alpha\right]\|\mathbf{n}\|=0\end{aligned} \tag{74}$$

but $\|\mathbf{n}\|\neq 0$, and thus

$$\gamma\|\boldsymbol{\Sigma}^*\|-2\gamma\langle\mu\rangle\bar{\Lambda}-\gamma\sqrt{\frac{2}{3}}\Delta H_\alpha-\sqrt{\frac{2}{3}}K_\alpha=0. \tag{75}$$

Differentiating this with respect to the deviatoric strain, $\mathbf{E}$, yields an implicit expression for the derivative $\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}$ in the following form:

$$\begin{aligned}&\gamma\frac{\partial\|\boldsymbol{\Sigma}^*\|}{\partial\mathbf{E}}-2\gamma\langle\mu\rangle\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}-\sqrt{\frac{2}{3}}\frac{\partial K_\alpha}{\partial\mathbf{E}}\\ &-\gamma\sqrt{\frac{2}{3}}\frac{\partial H_\alpha}{\partial\mathbf{E}}=\gamma\frac{1}{2}(\boldsymbol{\Sigma}^*:\boldsymbol{\Sigma}^*)^{-\frac{1}{2}}2\boldsymbol{\Sigma}^*\frac{\partial\boldsymbol{\Sigma}^*}{\partial\mathbf{E}}\\ &-2\gamma\langle\mu\rangle\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}-\frac{2}{3}K'_\alpha\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}-\sqrt{\frac{2}{3}}\frac{\partial K_\alpha}{\partial\dot{E}^{eq}}\frac{\partial\dot{E}^{eq}}{\partial\mathbf{E}}\\ &-\gamma\frac{2}{3}H'_\alpha\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}-\gamma\sqrt{\frac{2}{3}}\frac{\partial H_\alpha}{\partial\dot{E}^{eq}}\frac{\partial\dot{E}^{eq}}{\partial\mathbf{E}}\\ &=\gamma\frac{\boldsymbol{\Sigma}^*}{\|\boldsymbol{\Sigma}^*\|}2\langle\mu\rangle-2\gamma\langle\mu\rangle\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}-\frac{2}{3}K'_\alpha\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}\\ &-\sqrt{\frac{2}{3}}K^r_\alpha\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}-\gamma\frac{2}{3}H'_\alpha\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}\\ &-\gamma\sqrt{\frac{2}{3}}H^r_\alpha\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}=0\end{aligned}$$

which after rearrangement can be written as

$$\begin{aligned}&\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}\left[2\gamma\langle\mu\rangle+\frac{2}{3}(K'_\alpha+\gamma H'_\alpha)\right]\\ &=2\langle\mu\rangle\gamma\mathbf{n}-\sqrt{\frac{2}{3}}\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}(K^r_\alpha+\gamma H^r_\alpha),\end{aligned}$$

and finally the required derivative is

$$\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}=\frac{\gamma\langle\mu\rangle\mathbf{n}-\sqrt{\frac{1}{6}}\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}(K^r_\alpha+H^r_\alpha)}{\gamma\langle\mu\rangle+\frac{1}{3}(K'_\alpha+\gamma H'_\alpha)} \tag{76}$$

Using the derivatives expressed by Eqs. (70), (71), (72) and the final form of $\frac{\partial\bar{\Lambda}}{\partial\mathbf{L}}$ the stress-strain tangent modulus can be defined by

$$\begin{aligned}\left.\frac{\partial\mathbf{T}}{\partial\mathbf{L}}\right|_{n+1} &= \langle\kappa\rangle\mathbf{1}\otimes\mathbf{1}+\mathbf{n}\otimes\left[\hat{\mathbf{I}}_{dev}:\frac{2}{3}H'_\alpha\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}\right.\\ &\left.+\sqrt{\frac{2}{3}}H^r_\alpha\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}\right]_{n+1}\\ &+\bar{\gamma}\hat{\mathbf{I}}_{dev}:\left[2\langle\mu\rangle\hat{\mathbf{I}}-2\langle\mu\rangle\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}\otimes\mathbf{n}\right.\\ &\left.-\left\{\frac{2}{3}H'_\alpha\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}+\sqrt{\frac{2}{3}}H^r_\alpha\frac{1}{2}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}\right\}\otimes\mathbf{n}\right]_{n+1}\end{aligned}$$

$$+\mathbf{n}\otimes\left[\hat{\mathbf{I}}_{dev}:\frac{2}{3}K'_\alpha\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}+\sqrt{\frac{2}{3}}K^r_\alpha\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}\right]_{n+1}$$

$$= \langle\kappa\rangle\mathbf{1}\otimes\mathbf{1}+\left.\frac{\partial\bar{\Lambda}}{\partial\mathbf{E}}\right|_{n+1}\otimes\left[\hat{\mathbf{I}}_{dev}:\frac{2}{3}H'_\alpha\mathbf{n}+\right.$$

$$\hat{\mathbf{I}}_{dev}:\frac{2}{3}K'_\alpha\mathbf{n}-\bar{\gamma}2\langle\mu\rangle\hat{\mathbf{I}}_{dev}:\mathbf{n}$$

$$\left.-\frac{2}{3}\bar{\gamma}H'_\alpha\hat{\mathbf{I}}_{dev}:\mathbf{n}\right]_{n+1}$$

$$+\left[\bar{\gamma}\hat{\mathbf{I}}_{dev}2\langle\mu\rangle+(1-\gamma)H^r_\alpha\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}\otimes\mathbf{n}\right.$$

$$\left.+K^r_\alpha\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}\otimes\mathbf{n}\right]_{n+1}.$$

and after grouping scalars multiplying ($\hat{\mathbf{I}}_{dev}:\mathbf{n}$), can be written as

$$\left.\frac{\partial\mathbf{T}}{\partial\mathbf{L}}\right|_{n+1}=\langle\kappa\rangle\mathbf{1}\otimes\mathbf{1}$$

$$+\left[\frac{\gamma\langle\mu\rangle\mathbf{n}}{\gamma\langle\mu\rangle+\frac{1}{3}(K'_\alpha+\gamma H'_\alpha)}\right]\otimes$$

$$\left\{\hat{\mathbf{I}}_{dev}:\mathbf{n}\left[\frac{2}{3}[(1-\bar{\gamma})H'_\alpha+K'_\alpha]-\bar{\gamma}2\langle\mu\rangle\right]\right\}_{n+1}$$

$$+\left[\bar{\gamma}\hat{\mathbf{I}}_{dev}2\langle\mu\rangle+(1-\gamma)H^r_\alpha\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}\otimes\mathbf{n}\right.$$

$$\left.+K^r_\alpha\frac{1}{\Delta t}\frac{\Delta\mathbf{E}}{\Delta E^{eq}}\otimes\mathbf{n}\right]_{n+1}. \qquad (77)$$

3.2.3 Transformation Plasticity

The multiphase alloy, which is subjected to both internal stress and external loading, undergoes plastic deformations for the lower applied stress than the yield stress. This can happen due to the superposition of external and internal stresses. Internal stresses are generated mainly during phase transformations because of the variation of fraction specific volumes. The plastic yielding occurs in the direction of the applied stress.

The constitutive equation for transformation plasticity is based on the Levy-Mises perfectly plastic equation, and has been proposed by Greenwood and Johnson [6] in the following form:

$$\dot{E}^{trip}=\frac{5}{6}\frac{\mathbf{S}_{ex}}{Y}\frac{\dot{V}}{V}, \qquad (78)$$

where $\mathbf{S}_{ex}$ is the applied external stress, Y is the yield stress of the weaker phase of two phases: the daughter and parent, $\frac{\dot{V}}{V}$ is the rate of the specific volume change. Substituting $\frac{\dot{V}}{V}=3\,tr\dot{\mathbf{E}}_i^{tr}$ into Eq.(78) gives the constitutive equation for the transformation induced plasticity shown in [18], and written as

$$\dot{\mathbf{E}}^{trip}=\frac{5}{2}\frac{tr\dot{\mathbf{E}}_i^{tr}}{Y}\mathbf{S}_{ex}. \qquad (79)$$

where $tr\dot{\mathbf{E}}_i^{tr}$ is the trace of the transformation strain rate for phase i. The modification of this relation, presented in [2], can be expressed by

$$\dot{E}^{trip}_{IJ}=\frac{3}{2}\frac{\dot{E}^{trip}_{eq}}{S^{eq}}\Sigma_{IJ}, \qquad (80)$$

where the equivalent transformation induced plastic strain rate is defined by

$$\dot{E}^{trip}_{eq}=\left(\frac{2}{3}\dot{E}^{trip}_{IJ}\dot{E}^{trip}_{IJ}\right)^{\frac{1}{2}}. \qquad (81)$$

Assuming that the softer phase is rigid-ideal plastic, the constitutive equation for the transformation induced plastic strain rate can be expressed in the form:

$$\dot{E}^{trip}_{IJ}=K\,(1-y_i)\,\dot{y}_i\,\Sigma_{IJ}, \qquad (82)$$

which relates explicitly a portion of plastic strain rate with the phase fraction y_i and its rate $\dot{y}_i$.

This has been experimentally verified in [3] for steel with temperature $M_s=275C$, the material constant $K=1.5\times10^{-10}\left[\frac{m^2}{N}\right]$, and the austenite yield limit equal to 170 $\left[\frac{MN}{m^2}\right]$.

In the formulation of the TMM problem the volume phase fractions are also state variables and they are stored in a column vector, $\underline{y}$, with the position in the vector determined by a type of phase evolution. Eq. (82) can be written in the vector form

$$\dot{\mathbf{E}}^{trip}=K(\underline{1}-\underline{y}):\dot{\underline{y}}\,\mathbf{\Sigma} \qquad (83)$$

which is required for a consistent mathematical approach to the solution of TMM problem by FEM. The unit vector $\underline{1}=[1,1,1,...1]^T$ contains the same number of entries as the number of considered phase transformations. The symbol " :" indicates an inner product of vectors.

The trace of strain increment related to transformation plasticity is expressed by

$$\mathrm{tr}\Delta\mathbf{L}^{tp}=\underline{\alpha}:\Delta\underline{y}. \qquad (84)$$

4. FE Approximation of TMM Problem

The alloy with microstructure is approximated by super-elements, which correspond to grains, and are composed of several ordinary finite elements that contain various microregions or phases represented at elemental integration points, ie. nodes of Gaussian quadrature at elements. This hierarchy in the approximation of material properties is consistent with the micromechanical model of the alloy and provides for the transmission of information about micro-material state to the macro-level of finite element method solution.

The Finite Element Method for the fully coupled thermo-mechanical problem is based on Galerkin's approximation of variational equations i.e. the principle of virtual work and the balance of internal energy. The FEM consists of the following steps [1], [7]:

- The first step in developing the method is to construct the finite-dimensional approximation of the collections of trial functions $\mathcal{U}$ and the weighting functions $\mathcal{V}$, or variations, which are defined by

$$\mathcal{U}^h \subset \mathcal{U} \tag{85}$$
$$\textbf{if}\, u^h,\, \theta^h \;\in \mathcal{U}^h\, \textbf{then}\, u^h,\, \theta^h \;\in \mathcal{U}$$

$$\mathcal{V}^h \subset \mathcal{V} \tag{86}$$
$$\textbf{if}\, v^h;\, \vartheta^h \;\in \mathcal{V}^h\, \textbf{then}\, v^h,\, \vartheta^h \;\in \mathcal{V}$$

- Discretization of the space-time domain, $\Omega = \{(\mathbf{X},t); \mathbf{X} \in V, t \in [t_i, t_f]\}$, by a combination of finite elements, covering the space, and Euler finite differences through time. Discretizations are characterized by length scales $\{h_X, h_t\}$, correspondingly.
- Express v^h and ϑ^h as linear combinations of given shape functions, or interpolation functions,
- Approximation of integrals in variational equations by sums,
- Formulation of a coupled system of linear algebraic equations, usually expressed in the matrix form and called the **Finite Element Equation**, for values of v^h and ϑ^h at nodal points,
- Solution of the system of algebraic equations by the Newton-Raphson method.

The FE approximation of balance laws is combined with finite difference approximation of phase evolution law.

4.1 FE Approximation of Virtual Work Balance

The equation of virtual work Eq(37) is solved by the Finite Element Method combined with linearization techniques for **Finite Element Equation**. The linearizations are applied after incremental decompositions for strain and stress given by

$$^{t+\Delta t}\tilde{\mathbf{L}} = {}^{t}\tilde{\mathbf{L}} + \tilde{\mathbf{L}}^{\vartriangle} \tag{87}$$

$$^{t+\Delta t}\mathbf{T} = {}^{t}\mathbf{T} + \mathbf{T}^{\vartriangle} \tag{88}$$

where $^{t+\Delta t}\{\tilde{\mathbf{L}}, \mathbf{T}\}$ and $^{t}\{\tilde{\mathbf{L}}, \mathbf{T}\}$ corresponds to the actual and the previous strain-stress state. The increments of strain and stress are $\tilde{\mathbf{L}}^{\vartriangle}$, $\mathbf{T}^{\vartriangle}$. The increment of the Green-Lagrange strain $\tilde{\mathbf{L}}^{\vartriangle}$ is further decomposed into its linear and nonlinear components:

$$\tilde{\mathbf{L}}^{\vartriangle} = \tilde{\mathbf{L}} + \tilde{\mathbf{L}}_{\nu} \tag{89}$$

where

$$\tilde{\mathbf{L}} = \frac{1}{2}\left[\mathbf{F}^{\mathrm{T}} \cdot (\nabla \Delta \mathbf{u})^{\mathrm{T}} + (\nabla \Delta \mathbf{u} \cdot \mathbf{F})\right];$$
$$\tilde{\mathbf{L}}_{\nu} = \frac{1}{2} \nabla \Delta \mathbf{u} \, (\nabla \Delta \mathbf{u})^{\mathrm{T}}. \tag{90}$$

The finite element equation for virtual work, shown in [1], and [7], for the **total Lagrangian formulation** at time $(n+1)$ is obtained from Eq.(37) and expressed by

$$\left({}_0^t\mathbf{K}_L + {}_0^t\mathbf{K}_{nL}\right) \Delta \mathbf{u}^{(i)} = {}_0^{t+\Delta t}\mathbf{R}_u - {}_0^{t+\Delta t}\mathbf{F}_u^{(i-1)} \tag{91}$$

where ${}_0^t\mathbf{K}_L$ and ${}_0^t\mathbf{K}_{nL}$ is linear and nonlinear stiffness matrix, $\Delta \mathbf{u}^{(i)}$ is the vector of displacement increment, ${}_0^{t+\Delta t}\mathbf{R}_u$ is the vector of externally applied nodal point loads, ${}_0^{t+\Delta t}\mathbf{F}_u^{(i-1)}$ is the vector of nodal point forces equivalent to the internal stresses. This equation is linear in respect of $\Delta \mathbf{u}^{(i)}$ and the matrices in Eq.(91) are taken at four levels of solution. These matrices are evaluated at two time steps t and $(t+\Delta t)$, and for two iterations i and $(i-1)$. The linear stiffness matrix is defined by

$${}_0^t\mathbf{K}_L = \int_{V_0} {}_0^t\mathbf{B}_L^{\mathrm{T}} \; \mathbf{C}_{TL} \; {}_0^t\mathbf{B}_L \, dV_0 \tag{92}$$

where meaning of matrices ${}_0^t\mathbf{B}_L$ and $\mathbf{C}_{TL}$ comes from the following expression:

$$\left({}_0^t\mathbf{B}_L^{\mathrm{T}} \, \Delta \mathbf{u}^{\mathrm{T}}\right) \mathbf{C}_{TL} \left({}_0^t\mathbf{B}_L \Delta \mathbf{u}\right) = \tilde{\mathbf{L}}^{\mathrm{T}} : \mathbf{C}_{TL} : \tilde{\mathbf{L}}. \tag{93}$$

The matrix $\mathbf{C}_{TL}$ is the consistent or algorithmic tangent modulus which has to be defined for each material model as the $\left[\frac{\partial \mathbf{T}}{\partial \mathbf{L}}\right]$ contribution to the global stiffness matrix, and ${}_0^t\mathbf{B}_L$ is the linear strain-displacement matrix. The nonlinear stiffness matrix is defined by

$${}_0^t\mathbf{K}_{nL} = \int_{V_0} {}_0^t\mathbf{B}_{nL}^{\mathrm{T}} \; \mathbf{S}^{[mx]} \; {}_0^t\mathbf{B}_{nL} \, dV_0. \tag{94}$$

The sense of the nonlinear strain-displacement matrix ${}_0^t\mathbf{B}_{nL}$ comes from the substitution

$$\left({}_0^t\mathbf{B}_{nL}^{\mathrm{T}} \, \Delta \mathbf{u}^{\mathrm{T}}\right) \mathbf{S}^{[mx]} \left({}_0^t\mathbf{B}_{nL} \Delta \mathbf{u}\right) = \mathbf{S} : \tilde{\mathbf{L}}_{\nu}, \tag{95}$$

where $\mathbf{S}^{[mx]}$ is the matrix representation of 2nd Piola-Kirchhoff stress, ${}^t\mathbf{S}$. The linear and nonlinear stiffness matrices are not modified in iteration process during the step $(t+\Delta t)$. They are updated when the iteration process at $(t+\Delta t)$ is completed. The vector of externally applied nodal point loads is given by

$${}_0^{t+\Delta t}\mathbf{R}_u = \int_{\partial V_0} \mathbf{H}_s^{\mathrm{T}} \; {}^{t+\Delta t}\mathbf{T} d\mathcal{P} + \int_{V_0} \mathbf{H}^{\mathrm{T} t+\Delta t}\mathbf{b} \, dV_0 \tag{96}$$

where $\mathbf{H}_s$ is the surface interpolation matrix, and $\mathbf{H}$ is the volume interpolation matrix. These matrices are formed from the interpolating polynomial during the process of Gaussian integration. The matrix $\mathbf{H}_s$ is evaluated for two of the 3-coordinates at Gauss points and one at the given surface. The nominal stress vector is ${}^{t+\Delta t}\mathbf{T} = \{T_J\}$, and the vector of body forces is ${}^{t+\Delta t}\mathbf{b} = \{b_J\}$. The vector of nodal point forces equivalent to stresses at time $(t+\Delta t)$ and defined for previous iteration $(i-1)$ is expressed in the form

$$ {}^{t+\Delta t}_{0}\mathbf{F}_u^{(i-1)} = \int_{V_0} {}^{t}_{0}\mathbf{B}_L \; {}^{t+\Delta t}_{0}\tilde{\mathbf{S}}^{(i-1)} \, dV_0 \qquad (97) $$

4.2 FE Approximation of Internal Energy Balance

The variational equation of internal energy balance Eq.(38) is solved by the Galerkin type Finite Element Method. The appropriate finite element equation for the fully coupled thermo-mechanical problem is given by:

$$ {}^{t}_{0}\mathbf{C} \; {}^{t+\Delta t}_{0}\dot{\theta}^{(i)} + \left({}^{t}_{0}\mathbf{K}^k + {}^{t}_{0}\mathbf{K}^M + {}^{t}_{0}\mathbf{K}^r + {}^{t}_{0}\mathbf{K}^\rho\right) \Delta\theta^{(i)} $$
$$ = {}^{t+\Delta t}_{0}\mathbf{R}_\theta{}^{(i-1)} - {}^{t+\Delta t}_{0}\mathbf{R}_\Gamma^{(i-1)} - {}^{t+\Delta t}_{0}\mathbf{R}_{su}^{(i-1)} $$
$$ - {}^{t+\Delta t}_{0}\mathbf{R}_\Sigma^{(i-1)} - {}^{t+\Delta t}_{0}\mathbf{F}_{neq}^{(i-1)} - {}^{t+\Delta t}_{0}\mathbf{F}^\rho, \qquad (98) $$

where ${}^{t}_{0}\mathbf{K}^k$ is the stiffness matrix corresponding to conduction, ${}^{t}_{0}\mathbf{K}^M$ is the stiffness related to the heat generated by mechanical energy, ${}^{t}_{0}\mathbf{K}^r$ is the stiffness resulting from entropy radiation, ${}^{t}_{0}\mathbf{K}^\rho$ and ${}^{t+\Delta t}_{0}\mathbf{F}^\rho$ are related to the dissipation of inelastic energy $(\mathbf{E}^{pl} : \mathbf{S})$, and ${}^{t+\Delta t}_{0}\mathbf{F}_{neq}^{(i-1)}$ is called the matrix of non-equilibrated heat fluxes generated due to convergence criterion applied in iteration technique. The R.H.S. vector of nodal thermal loads, which correspond to the thermal boundary conditions, is given by

$$ {}^{t+\Delta t}_{0}\mathbf{R}_\theta^{(i-1)} = {}^{t+\Delta t}_{0}\mathbf{R}_\theta^{k\,(i-1)} + {}^{t+\Delta t}_{0}\mathbf{R}_\theta^{c\,(i-1)} + {}^{t+\Delta t}_{0}\mathbf{R}_\theta^{r\,(i-1)} \qquad (99) $$

where $\mathbf{R}_\theta^k, \mathbf{R}_\theta^c, \mathbf{R}_\theta^r$ are fluxes due to conduction, convection and radiation phenomena on external surfaces of the body. The terms ${}^{t+\Delta t}_{0}\mathbf{R}_\Gamma^{(i-1)}$ and ${}^{t+\Delta t}_{0}\mathbf{R}_{su}^{(i-1)}$ are connected with internal heat fluxes generated in the thickest FE region containing the singular surface $\partial\Gamma^{pt}$ or separate microregions, where thermally activated phase transformations proceed. The correspondence of terms appearing in Eq.(98) has been summarized in **Table 4.2**.

The FE Eq.(98) can be written in the form consistent with the FE virtual work Eq.(91)

$$ {}^{t}_{0}\mathbf{C} \; {}^{t+\Delta t}_{0}\dot{\theta}^{(i)} + $$
$$ \left({}^{t}_{0}\mathbf{K}^k + {}^{t}_{0}\mathbf{K}^M + {}^{t}_{0}\mathbf{K}^r + {}^{t}_{0}\mathbf{K}^\rho\right) \Delta\theta^{(i)} $$
$$ = {}^{t+\Delta t}_{0}\mathbf{R}_\theta{}^{(i-1)} - {}^{t+\Delta t}_{0}\mathbf{F}_\theta^{(i-1)}, \qquad (100) $$

when substituting the matrix of residual fluxes given by

$$ {}^{t+\Delta t}_{0}\mathbf{F}_\theta^{(i-1)} = {}^{t+\Delta t}_{0}\mathbf{R}_\Gamma^{(i-1)} + {}^{t+\Delta t}_{0}\mathbf{R}_{su}^{(i-1)} $$
$$ + {}^{t+\Delta t}_{0}\mathbf{R}_\Sigma^{(i-1)} + {}^{t+\Delta t}_{0}\mathbf{F}_{neq}^{(i-1)} + {}^{t+\Delta t}_{0}\mathbf{F}^\rho. \qquad (101) $$

Table 1 Correspondence of matrices in FE equation for thermo-mechanical problem and integrals in the balance of internal energy.

FE Eq.(98)	Energy Eq.(38)	Meaning
${}^{t}_{0}\mathbf{C}\;{}^{t+\Delta t}_{0}\dot{\theta}^{(i)}$	$-\int_{V_0} c\dot{\theta}\;\delta\vartheta dV$	"heat energy"
${}^{t}_{0}\mathbf{K}^k\Delta\theta^{(i)}$	$\int_{V_0} k_{IJ}\theta_{,I}\;\delta\vartheta_{,J}dV$	heat flux
${}^{t}_{0}\mathbf{K}^M\Delta\theta^{(i)}$	$\int_{V_0} f_\theta^M\;\delta\vartheta dV$	mech. energy
${}^{t}_{0}\mathbf{K}^r\Delta\theta^{(i)}$	$\int_{V_0} f_\theta^r\;\delta\vartheta dV$	entropy radia.
${}^{t+\Delta t}_{0}\mathbf{R}_\theta^{kcr(i-1)}$	$\int_{\partial V_0} f_\theta^{\partial V}\;\delta\vartheta d\mathcal{P}$	bound. fluxes
${}^{t+\Delta t}_{0}\mathbf{R}_\Gamma^{(i-1)}$	$\int_{\partial\Gamma^{pt}} f_\theta^{su}\;\delta\vartheta d\mathcal{P}$	surf. energy
${}^{t+\Delta t}_{0}\mathbf{R}_{su}^{(i-1)}$	$\int_{\partial\Gamma^{pt}} f_\theta^{su}\;\delta\vartheta d\mathcal{P}$	energy jump
${}^{t+\Delta t}_{0}\mathbf{R}_\Sigma^{(i-1)}$	$\sum_{\mathcal{J}} \mathcal{F}_\theta^{\mathcal{J}}\delta\vartheta\mid_{\mathcal{J}}$	point source

5. FE Equation for TMM Problem

The assemblage of FE equations for virtual work Eq.(91) and internal energy Eq.(100) together with appropriate phase evolution law yields the combined **Global Finite Element Equation** for thermo-mechanical-metallurgical problem. The global FE equation for thermo-mechanical problem is formulated at first, and afterwards more complex thermo-mechanical-metallurgical problem will be presented.

5.1 Global FE Equation for TM Problem

The displacement increment $\Delta\mathbf{u}$ and temperature θ are state variables for the coupled thermo-mechanical problem which is defined by Eqs.(91) and (100). The corresponding global FE equation is expressed as the following:

$$ \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & {}^{t}_{0}\mathbf{C} \end{bmatrix} \begin{bmatrix} {}^{t+\Delta t}\dot{\mathbf{u}} \\ {}^{t+\Delta t}\dot{\theta} \end{bmatrix}^{(i)} + \begin{bmatrix} {}^{t}_{0}\mathbf{K}_{uu} & {}^{t}_{0}\mathbf{K}_{u\theta} \\ {}^{t}_{0}\mathbf{K}_{\theta u} & {}^{t}_{0}\mathbf{K}_{\theta\theta} \end{bmatrix} \begin{bmatrix} \Delta\mathbf{u} \\ \Delta\theta \end{bmatrix}^{(i)} = \begin{bmatrix} {}^{t+\Delta t}\mathbf{R}_u \\ {}^{t+\Delta t}\mathbf{R}_\theta \end{bmatrix} - \begin{bmatrix} {}^{t+\Delta t}_{0}\mathbf{F}_u \\ {}^{t+\Delta t}_{0}\mathbf{F}_\theta \end{bmatrix}^{(i-1)} \qquad (102) $$

where ${}^{t}_{0}\mathbf{K}_{uu}$ is the stiffness corresponding to mechanical effects, ${}^{t}_{0}\mathbf{K}_{u\theta}$ is the matrix which transforms thermal energy into mechanical and matrix ${}^{t}_{0}\mathbf{K}_{\theta u}$ transform mechanical energy into thermal, the thermal stiffness ${}^{t}_{0}\mathbf{K}_{\theta\theta}$ is a sum of ${}^{t}_{0}\mathbf{K}^k$, ${}^{t}_{0}\mathbf{K}^c$ and ${}^{t}_{0}\mathbf{K}^r$. The right hand vectors of Eq.(102) are defined by Eqs.(96), (97), (99), (101). The stiffness matrices ${}^{t}_{0}\mathbf{K}_{uu}$, ${}^{t}_{0}\mathbf{K}_{\theta\theta}$, ${}^{t}_{0}\mathbf{K}_{u\theta}$ and ${}^{t}_{0}\mathbf{K}_{\theta u}$ are defined by appropriate integrals with kernels expressed by a combination of unknowns $\{\Delta\mathbf{u}, \theta\}$, shape functions, and strain-displacement matrices, as has been shown in [13], [14].

They can be also viewed from the perspective of the Newton-Raphson solution process as the derivatives of vectors $\mathbf{F}_u$, $\mathbf{F}_\theta$ with respect to the state variable $\Delta\mathbf{u}$ and θ. Hence, they can be also expressed as follows:

$$\begin{aligned} {}^t_0\mathbf{K}_{uu} &= {}^t_0\mathbf{F}_{u,u}; \\ {}^t_0\mathbf{K}_{\theta\theta} &= {}^t_0\mathbf{F}_{\theta,\theta}; \\ {}^t_0\mathbf{K}_{u\theta} &= {}^t_0\mathbf{F}_{u,\theta}; \\ {}^t_0\mathbf{K}_{\theta u} &= {}^t_0\mathbf{F}_{\theta,u}, \end{aligned} \tag{103}$$

where ',' indicates differentiation.

The balance of internal energy expressed by Eq(100) for the temperature rate approximated by the backward Euler scheme can be written in the form

$$\left\{ \frac{1}{\Delta t} {}^t_0\mathbf{C} + {}^t_0\mathbf{K}^k + {}^t_0\mathbf{K}^c + {}^t_0\mathbf{K}^r + {}^t_0\mathbf{K}^\rho \right\} \Delta\theta^{(i)} = {}^{t+\Delta t}_0\mathbf{R}_\theta - {}^{t+\Delta t}_0\mathbf{F}_\theta^{(i-1)}. \tag{104}$$

Substituting this to Eq.(102), the global finite element equation for the thermo-mechanical system can be rewritten in a more compact form

$$\begin{bmatrix} {}^t_0\mathbf{K}_{uu} & {}^t_0\mathbf{K}_{u\theta} \\ {}^t_0\mathbf{K}_{\theta u} & \frac{1}{\Delta t} {}^t_0\mathbf{C} + {}^t_0\mathbf{K}_{\theta\theta} \end{bmatrix} \begin{bmatrix} \Delta\mathbf{u} \\ \Delta\theta \end{bmatrix}^{(i)} = \begin{bmatrix} {}^{t+\Delta t}\mathbf{R}_u \\ {}^{t+\Delta t}\mathbf{R}_\theta \end{bmatrix} - \begin{bmatrix} {}^{t+\Delta t}_0\mathbf{F}_u \\ {}^{t+\Delta t}_0\mathbf{F}_\theta \end{bmatrix}^{(i-1)} \tag{105}$$

where matrix ${}^t_0\mathbf{K}_{\theta\theta}$ is defined by

$${}^t_0\mathbf{K}_{\theta\theta} = {}^t_0\mathbf{K}^k + {}^t_0\mathbf{K}^c + {}^t_0\mathbf{K}^r + {}^t_0\mathbf{K}^\rho. \tag{106}$$

5.2 Global FE Equation for Body with Phase Transformations

Combining Eq.(102) together with evolution equation for ferritic and pearlitic transformations, shown in Table 5 of Part1, the following global FE equation is obtained:

$$\begin{bmatrix} -\mathbf{1} & {}^t\hat{\mathcal{B}}_i & {}^t\mathcal{A}_i \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & {}^t_0\mathbf{C} \end{bmatrix} \begin{bmatrix} {}^{t+\Delta t}\dot{\mathbf{y}}_i \\ {}^{t+\Delta t}\dot{\mathbf{u}} \\ {}^{t+\Delta t}\dot{\theta} \end{bmatrix}^{(i)} + \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ {}^t_0\mathbf{K}_{uy} & {}^t_0\mathbf{K}_{uu} & {}^t_0\mathbf{K}_{u\theta} \\ {}^t_0\mathbf{K}_{\theta y} & {}^t_0\mathbf{K}_{\theta u} & {}^t_0\mathbf{K}_{\theta\theta} \end{bmatrix} \begin{bmatrix} \Delta\mathbf{y}_i \\ \Delta\mathbf{u} \\ \Delta\theta \end{bmatrix}^{(i)} = \begin{bmatrix} {}^{t+\Delta t}\mathbf{R}_{y_i} \\ {}^{t+\Delta t}\mathbf{R}_u \\ {}^{t+\Delta t}\mathbf{R}_\theta \end{bmatrix} - \begin{bmatrix} {}^{t+\Delta t}_0\mathbf{F}_{y_i} \\ {}^{t+\Delta t}_0\mathbf{F}_u \\ {}^{t+\Delta t}_0\mathbf{F}_\theta \end{bmatrix}^{(i-1)} \tag{107}$$

where the vector ${}^{t+\Delta t}\mathbf{R}_{y_i}$ is related to the term $\mathcal{R}_i$ of Eq.(154), components of stiffness matrix: ${}^t_0\mathbf{K}_{uu}$, ${}^t_0\mathbf{K}_{u\theta}$, ${}^t_0\mathbf{K}_{\theta u}$, and ${}^t_0\mathbf{K}_{\theta\theta}$, as well as the RHS vectors: ${}^{t+\Delta t}_0\mathbf{F}_u{}^{(i-1)}$, ${}^{t+\Delta t}_0\mathbf{F}_\theta{}^{(i-1)}$, ${}^{t+\Delta t}_0\mathbf{R}_u$, ${}^{t+\Delta t}_0\mathbf{R}_\theta$, are the same as in Eq.(102), and the subscript i assumes two values: 2 for ferritic, and 3 for pearlitic transformation.

Approximating the fraction rate, velocity, and temperature rate by backward finite differences, the system of FE equations can be written in the following form:

$$\begin{bmatrix} {}^t_0\mathbf{K}_{yy} & {}^t_0\mathbf{K}_{yu} & {}^t_0\mathbf{K}_{y\theta} \\ {}^t_0\mathbf{K}_{uy} & {}^t_0\mathbf{K}_{uu} & {}^t_0\mathbf{K}_{u\theta} \\ {}^t_0\mathbf{K}_{\theta y} & {}^t_0\mathbf{K}_{\theta u} & {}^t_0\hat{\mathbf{K}}_{\theta\theta} \end{bmatrix} \begin{bmatrix} \Delta\mathbf{y}_i \\ \Delta\mathbf{u} \\ \Delta\theta \end{bmatrix}^{(i)} = \begin{bmatrix} {}^{t+\Delta t}\mathbf{R}_{y_i} \\ {}^{t+\Delta t}\mathbf{R}_u \\ {}^{t+\Delta t}\mathbf{R}_\theta \end{bmatrix} - \begin{bmatrix} {}^{t+\Delta t}_0\mathbf{F}_{y_i} \\ {}^{t+\Delta t}_0\mathbf{F}_u \\ {}^{t+\Delta t}_0\mathbf{F}_\theta \end{bmatrix}^{(i-1)} \tag{108}$$

with $\tau = \frac{1}{\Delta t}$, and stiffness matrices defined as such

$$\begin{aligned} {}^t_0\mathbf{K}_{yy} &= -\tau\,\mathbf{1}; \\ {}^t_0\mathbf{K}_{yu} &= \tau\,{}^t\hat{\mathcal{B}}_i; \\ {}^t_0\mathbf{K}_{y\theta} &= \tau\,{}^t\mathcal{A}_i; \\ {}^t_0\mathbf{K}_{uy} &= {}^t_0\mathbf{K}_\Lambda; \\ {}^t_0\mathbf{K}_{\theta y} &= {}^t_0\mathbf{K}_{mix}; \\ {}^t_0\hat{\mathbf{K}}_{\theta\theta} &= \tau\,{}^t_0\mathbf{C} + {}^t_0\mathbf{K}_{\theta\theta}, \end{aligned} \tag{109}$$

where ${}^t_0\mathbf{K}_\Lambda$ is related to the plastic function $\Lambda(\mathbf{S}, \mathbf{E}, \int \dot{\mathbf{E}}dt, \theta, y_i)$ and FE displacement-strain matrices $\mathbf{B}_L$, $\mathbf{B}_{nL}$, the stiffness matrix ${}^t_0\mathbf{K}_{mix}$ depends on the mixture rule used to evaluate material parameters for multiphase body.

The kinetic law for bainitic transformation, expressed by Eq.(37) of Part 1, reveals that this phase growth is not related to temperature rate nor to displacement velocity $\dot{\mathbf{u}}$. Therefore the rate of bainitic phase fraction $\dot{\mathbf{y}}_4^\phi$ is not coupled explicitly with other two state variables: $\Delta\mathbf{u}$, $\Delta\theta$, and the thermo-mechanical-metallurgical problem is described by Eq.(37) of Part 1 and Eq.(102) or Eq.(105).

The thermo-mechanical-metallurgical problem with martensitic transformation is described by the global FE Eq.(108) taken with matrices

$$\begin{aligned} {}^t_0\mathbf{K}_{yu} &= \tau\,{}^t\hat{\mathcal{B}}_6; \\ {}^t_0\mathbf{K}_{y\theta} &= \tau\,{}^t\mathcal{A}_6, \end{aligned} \tag{110}$$

and R.H.S. vectors evaluated appropriately for this reaction, i.e. ${}^{t+\Delta t}_0\mathbf{F}_{y_6}$ and ${}^{t+\Delta t}\mathbf{S}_{y_6}$. These matrices and vectors are derived correspondingly to factors of equation shown in Table 4 of Part 1.

6. Solution of FE Equations

The nonlinear finite element system of equations given either by Eq.(105) or Eq.(108) is solved iteratively by the Newton-Raphson scheme. The system Eq.(108) can be rewritten in the form

$$[\mathcal{K}]\,[\mathcal{U}] = [\mathcal{R}] - [\mathcal{F}] \tag{111}$$

where

$$[\mathcal{K}] = \begin{bmatrix} {}^t_0\mathbf{K}_{yy} & {}^t_0\mathbf{K}_{yu} & {}^t_0\mathbf{K}_{y\theta} \\ {}^t_0\mathbf{K}_{uy} & {}^t_0\mathbf{K}_{uu} & {}^t_0\mathbf{K}_{u\theta} \\ {}^t_0\mathbf{K}_{\theta y} & {}^t_0\mathbf{K}_{\theta u} & {}^t_0\hat{\mathbf{K}}_{\theta\theta} \end{bmatrix}; \tag{112}$$

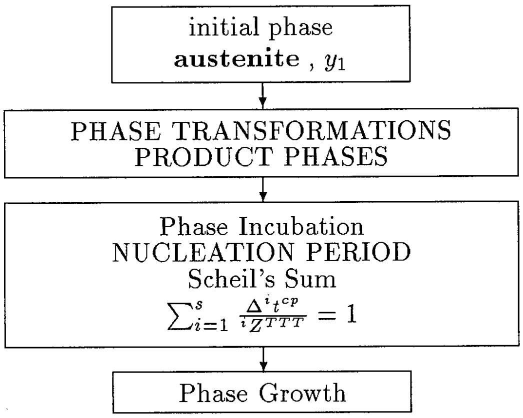

Fig 1 Nucleation and solid phase transformations

$$[\mathcal{U}] = \begin{bmatrix} \Delta \mathbf{y}_j \\ \Delta \mathbf{u} \\ \Delta \theta \end{bmatrix}^{(i)} ; \tag{113}$$

$$[\mathcal{F}] = \begin{bmatrix} {}_0^{t+\Delta t}\mathbf{F}_y \\ {}_0^{t+\Delta t}\mathbf{F}_u \\ {}_0^{t+\Delta t}\mathbf{F}_\theta \end{bmatrix}^{(i-1)} ; \tag{114}$$

$$[\mathcal{R}] = \begin{bmatrix} {}^{t+\Delta t}\mathbf{R}_y \\ {}^{t+\Delta t}\mathbf{R}_u \\ {}^{t+\Delta t}\mathbf{R}_\theta \end{bmatrix} ; \tag{115}$$

The L.H.S. can be defined as the linear function of $[\mathcal{U}]$

$$f\,[\mathcal{U}] = [\mathcal{K}]\,[\mathcal{U}] \tag{116}$$

The Newton-Raphson method provides the approximation $[\mathcal{U}]^{i+1}$ of the root $[\mathcal{U}]^*$ of the equation

$$f\,[\mathcal{U}] = 0 \tag{117}$$

computed from the approximation $[\mathcal{U}]^i$ using the equation

$$[\mathcal{U}]^{i+1} = [\mathcal{U}]^i - [\mathcal{K}]^{-1}\left([\mathcal{R}] - [\mathcal{F}]^i\right) \tag{118}$$

The recombination of the last relation leads to the form

$$[\mathcal{K}]\left([\mathcal{U}]^{i+1} - [\mathcal{U}]^i\right) = [\mathcal{F}]^i - [\mathcal{R}] \tag{119}$$

from where the convergence of the method can be evaluated. The matrix $[\mathcal{U}]^{i+1}$ converges to the solution $[\mathcal{U}]^*$ when $\left([\mathcal{U}]^{i+1} - [\mathcal{U}]^i\right)$ converges to zero that happens when the vector of nodal thermal and mechanical loads $[\mathcal{R}]$ balances the vector of nodal stress vectors and heat fluxes $[\mathcal{F}]^i$ i.e. $[\mathcal{F}]^i - [\mathcal{R}] = \mathbf{0}$.

7. Temperature-Displacement-Phase Fraction Coupling

The global stiffness matrix for TMM problem consists of terms which couple each of two state variables: temperature, displacement, and phase fractions. Submatrices will be derived here subsequently.

7.1 Displacement-temperature coupling

The finite element matrix $\mathbf{K}_{u\theta}$ coupling the displacement and temperature in Eq.(107) is defined in terms of stress derivatives by

$$\mathbf{K}_{u\theta} = \int_{V_0} \mathbf{B}_L^T \mathbf{C}_{T\theta}\, dV_0 \tag{120}$$

where the matrix

$$\mathbf{C}_{T\theta} = \left[\ \left(\frac{\partial \mathbf{T}}{\partial \theta}\right)_1 \ \left(\frac{\partial \mathbf{T}}{\partial \theta}\right)_2 \ \cdots \ \left(\frac{\partial \mathbf{T}}{\partial \theta}\right)_N\ \right] \tag{121}$$

consists of column vectors $\left(\frac{\partial \mathbf{T}}{\partial \theta}\right)_i$ of the dimension 6×1, and N is the number of nodes in the element.

These column vectors are calculated from the stress-temperature derivative which is evaluated using the same procedure as for derivation of $\left.\frac{\partial \mathbf{T}}{\partial \mathbf{L}}\right|_{n+1}$.

The stress-temperature derivative is expressed by

$$\begin{aligned} \left.\frac{\partial \mathbf{T}}{\partial \theta}\right|_{n+1} &= \\ &\frac{\partial}{\partial \theta}\Big\{\langle\kappa\rangle\left[\mathrm{tr}\Delta\mathbf{L} - \Delta t \underline{\alpha}^{tra} : \dot{\underline{y}} - \langle\alpha^{thm}\rangle\Delta\theta\right]\mathbf{1} \\ &+\mathbf{Z} + \sqrt{\frac{2}{3}}K_\alpha \mathbf{n} + 2\langle\mu\rangle\Delta t\dot{\mathbf{E}}^{trip}\Big\}_{n+1} \\ = \ &\langle\kappa\rangle_{,\theta}\left[\mathrm{tr}\Delta\mathbf{L} - \underline{\alpha}^{tra} : \Delta\underline{y} - \langle\alpha^{thm}\rangle\Delta\theta\right]_{n+1}\mathbf{1} \\ &-\langle\kappa\rangle\Big[(\underline{\alpha}^{tra}_{,\theta} : \Delta\underline{y} + \Delta t : \underline{\alpha}^{tra}\left\{\frac{\partial \dot{\underline{y}}}{\partial \theta} + \frac{\partial \dot{\underline{y}}}{\partial \mathbf{S}} : \frac{\partial \mathbf{S}}{\partial \theta}\right\} \\ &+(\alpha_{thm\,,\theta}\Delta\theta + \langle\alpha^{thm}\rangle)\Big]_{n+1}\mathbf{1} \end{aligned}$$

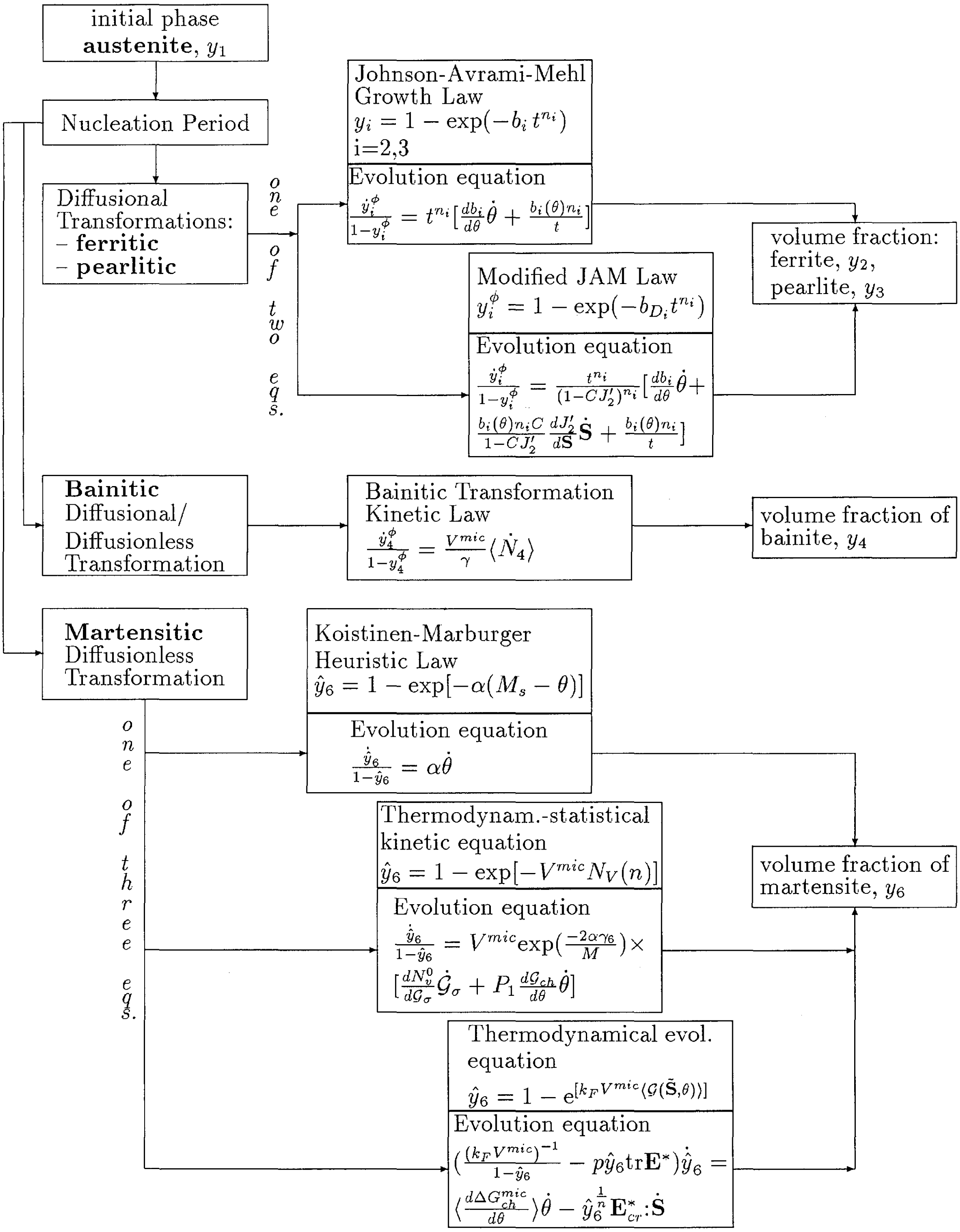

Fig 2 Phase transformations and evolution laws in steel

$$+ \left.\frac{\partial \mathbf{Z}}{\partial \theta}\right|_{n+1} + \left[\sqrt{\frac{2}{3}}K_{\alpha,\theta}\mathbf{n} + 2\langle\mu\rangle\Delta t\dot{\mathbf{E}}^{trip}_{,\theta}\right]_{n+1} \quad (122)$$

where the derivative of the transformation plasticity strain rate is

$$\frac{\partial \dot{\mathbf{E}}^{trip}}{\partial \theta} = K_{,\theta}(\underline{1} - \underline{y}) : \underline{\dot{y}}\boldsymbol{\Sigma} + K(\underline{1} - \underline{y}) : \left\{\frac{\partial \underline{\dot{y}}}{\partial \theta} + \frac{\partial \underline{\dot{y}}}{\partial \mathbf{S}} : \frac{\partial \mathbf{S}}{\partial \theta}\right\}\boldsymbol{\Sigma} + K(\underline{1} - \underline{y}) : \underline{\dot{y}}\,\frac{\partial \boldsymbol{\Sigma}}{\partial \theta} \quad (123)$$

The other derivatives required for evaluation of $\left.\frac{\partial \mathbf{T}}{\partial \theta}\right|_{n+1}$ are:

$$\frac{\partial \underline{\dot{y}}}{\partial \theta} + \frac{\partial \underline{\dot{y}}}{\partial \mathbf{S}} : \frac{\partial \mathbf{S}}{\partial \theta} = \frac{\partial \underline{\dot{y}}}{\partial \theta} + \frac{\partial \underline{\dot{y}}}{\partial \mathbf{S}} : \hat{\mathbf{I}}_{dev} : \frac{\partial \mathbf{T}}{\partial \theta}, \quad (124)$$

$$\frac{\partial \boldsymbol{\Sigma}}{\partial \theta} = \frac{\partial \boldsymbol{\Sigma}}{\partial \mathbf{S}} : \frac{\partial \mathbf{S}}{\partial \mathbf{T}} : \frac{\partial \mathbf{T}}{\partial \theta} = \hat{\mathbf{I}}_{dev} : \frac{\partial \mathbf{T}}{\partial \theta}, \quad (125)$$

and

$$\left.\frac{\partial \mathbf{Z}}{\partial \theta}\right|_{n+1} = \left[\sqrt{\frac{2}{3}}\frac{\partial H_\alpha}{\partial \theta}\mathbf{n}\right]_{n+1}. \quad (126)$$

Substituting these expressions to Eq.(122) yields

$$\begin{aligned}\left.\frac{\partial \mathbf{T}}{\partial \theta}\right|_{n+1} &= \langle\kappa\rangle_{,\theta}\left[\mathrm{tr}\Delta\mathbf{L} - \underline{\alpha}^{tra} : \Delta\underline{y} - \langle\alpha^{thm}\rangle\Delta\theta\right]_{n+1}\mathbf{1} - \langle\kappa\rangle\left[(\underline{\alpha}^{tra}_{,\theta} : \Delta t\underline{\dot{y}} + \Delta t\underline{\alpha}^{tra} : \left(\frac{\partial \underline{\dot{y}}}{\partial \theta} + \frac{\partial \underline{\dot{y}}}{\partial \mathbf{S}} : \hat{\mathbf{I}}_{dev} : \frac{\partial \mathbf{T}}{\partial \theta}\right)\right.\\ &\quad \left. + \left(\alpha^{thm}_{,\theta}\Delta\theta + \langle\alpha^{thm}\rangle\right)\right]_{n+1}\mathbf{1} + \left[\sqrt{\frac{2}{3}}H_{\alpha,\theta}\mathbf{n} + \sqrt{\frac{2}{3}}K_{\alpha,\theta}\mathbf{n}\right]_{n+1}\\ &\quad + 2\langle\mu\rangle\Delta t\left\{K_{,\theta}(\underline{1} - \underline{y}) : \underline{\dot{y}}\boldsymbol{\Sigma} + K(\underline{1} - \underline{y}) : \left(\frac{\partial \underline{\dot{y}}}{\partial \theta} + \frac{\partial \underline{\dot{y}}}{\partial \mathbf{S}} : \hat{\mathbf{I}}_{dev} : \frac{\partial \mathbf{T}}{\partial \theta}\right)\boldsymbol{\Sigma}\right.\\ &\quad \left. + K(\underline{1} - \underline{y}) : \underline{\dot{y}}\,\hat{\mathbf{I}}_{dev} : \left[\frac{\partial \mathbf{T}}{\partial \theta} - \sqrt{\frac{2}{3}}H_{\alpha,\theta}\mathbf{n}\right]\right\}_{n+1}\end{aligned}$$

that after rearrangement in respect to $\frac{\partial \mathbf{T}}{\partial \theta}$ gives the following:

$$\begin{aligned}&\left.\frac{\partial \mathbf{T}}{\partial \theta}\right|_{n+1} + \langle\kappa\rangle\Delta t\underline{\alpha}^{tra} : \frac{\partial \underline{\dot{y}}}{\partial \mathbf{S}} : \hat{\mathbf{I}}_{dev} : \left.\frac{\partial \mathbf{T}}{\partial \theta}\right|_{n+1}\mathbf{1} - 2\langle\mu\rangle\Delta t\left[K(\underline{1} - \underline{y}) : \frac{\partial \underline{\dot{y}}}{\partial \mathbf{S}} : \hat{\mathbf{I}}_{dev} : \frac{\partial \mathbf{T}}{\partial \theta}\right]_{n+1}\boldsymbol{\Sigma}_{n+1} + E^{trip}_{\alpha}\hat{\mathbf{I}}_{dev} : \left.\frac{\partial \mathbf{T}}{\partial \theta}\right|_{n+1}\\ &= \langle\kappa\rangle_{,\theta}\left[\mathrm{tr}\Delta\mathbf{L} - \underline{\alpha}^{tra} : \Delta\underline{y} - \langle\alpha^{thm}\rangle\Delta\theta\right]_{n+1}\mathbf{1} - \langle\kappa\rangle\left[(\underline{\alpha}^{tra}_{,\theta} : \Delta t\underline{\dot{y}} + \Delta t\underline{\alpha}^{tra} : \frac{\partial \underline{\dot{y}}}{\partial \theta} + \left(\alpha^{thm}_{,\theta}\Delta\theta + \langle\alpha^{thm}\rangle\right)\right]_{n+1}\mathbf{1}\\ &\quad + \left[\sqrt{\frac{2}{3}}H_{\alpha,\theta}\mathbf{n} + \sqrt{\frac{2}{3}}K_{\alpha,\theta}\mathbf{n}\right]_{n+1} + 2\langle\mu\rangle\Delta t\left[K_{,\theta}(\underline{1} - \underline{y}) : \underline{\dot{y}}\boldsymbol{\Sigma} + K(\underline{1} - \underline{y}) : \frac{\partial \underline{\dot{y}}}{\partial \theta}\boldsymbol{\Sigma} - E^{trip}_{\alpha}\hat{\mathbf{I}}_{dev} : \sqrt{\frac{2}{3}}H_{\alpha,\theta}\mathbf{n}\right]_{n+1}. \quad (127)\end{aligned}$$

The L.H.S. of Eq.(127) can be also expressed as a product of the fourth and the second order tensors and written in the following form:

$$\begin{aligned}&\left[\hat{\mathbf{I}} + \langle\kappa\rangle\Delta t\underline{\alpha}^{tra} : \frac{\partial \underline{\dot{y}}}{\partial \mathbf{S}} \otimes \mathbf{1} : \hat{\mathbf{I}}_{dev} - 2\langle\mu\rangle\Delta tK(\underline{1} - \underline{y}) : \frac{\partial \underline{\dot{y}}}{\partial \mathbf{S}} \otimes \boldsymbol{\Sigma} : \hat{\mathbf{I}}_{dev} + E^{trip}_{\alpha}\hat{\mathbf{I}}_{dev}\right]_{n+1} : \left.\frac{\partial \mathbf{T}}{\partial \theta}\right|_{n+1}\\ &= \langle\kappa\rangle_{,\theta}\left[\mathrm{tr}\Delta\mathbf{L} - \underline{\alpha}^{tra} : \Delta\underline{y} - \langle\alpha^{thm}\rangle\Delta\theta\right]\mathbf{1} - \langle\kappa\rangle\left[(\underline{\alpha}^{tra}_{,\theta} : \Delta t\,\underline{\dot{y}} + \Delta t\underline{\alpha}^{tra} : \frac{\partial \underline{\dot{y}}}{\partial \theta} + \left(\alpha^{thm}_{,\theta}\Delta\theta + \langle\alpha^{thm}\rangle\right)\right]_{n+1}\mathbf{1}\\ &\quad + \left[\sqrt{\frac{2}{3}}H_{\alpha,\theta}\mathbf{n} + \sqrt{\frac{2}{3}}K_{\alpha,\theta}\mathbf{n}\right]_{n+1} + 2\langle\mu\rangle\Delta t\left[K_{,\theta}(\underline{1} - \underline{y}) : \underline{\dot{y}}\boldsymbol{\Sigma} + K(\underline{1} - \underline{y}) : \frac{\partial \underline{\dot{y}}}{\partial \theta}\boldsymbol{\Sigma} - E^{trip}_{\alpha}\hat{\mathbf{I}}_{dev} : \sqrt{\frac{2}{3}}H_{\alpha,\theta}\mathbf{n}\right]_{n+1}. \quad (128)\end{aligned}$$

Finally the required stress-temperature derivative is given by

$$\begin{aligned}\left.\frac{\partial \mathbf{T}}{\partial \theta}\right|_{n+1} &= \left[\hat{\mathbf{I}} + \langle\kappa\rangle\Delta t\underline{\alpha}^{tra} : \frac{\partial \underline{\dot{y}}}{\partial \mathbf{S}} \otimes \mathbf{1} : \hat{\mathbf{I}}_{dev} - 2\langle\mu\rangle\Delta tK(\underline{1} - \underline{y}) : \frac{\partial \underline{\dot{y}}}{\partial \mathbf{S}} \otimes \boldsymbol{\Sigma} : \hat{\mathbf{I}}_{dev} + E^{trip}_{\alpha}\hat{\mathbf{I}}_{dev}\right]^{-1}_{n+1} :\\ &\quad \left\{\langle\kappa\rangle_{,\theta}\left[\mathrm{tr}\Delta\mathbf{L} - \underline{\alpha}^{tra} : \Delta\underline{y} - \langle\alpha^{thm}\rangle\Delta\theta\right]\mathbf{1} - \langle\kappa\rangle\left[(\underline{\alpha}^{tra}_{,\theta} : \Delta t\underline{\dot{y}} + \Delta t\underline{\alpha}^{tra} : \frac{\partial \underline{\dot{y}}}{\partial \theta} + \left(\alpha^{thm}_{,\theta}\Delta\theta + \langle\alpha^{thm}\rangle\right)\right]\mathbf{1}\right.\\ &\quad + \sqrt{\frac{2}{3}}H_{\alpha,\theta}\mathbf{n} + \sqrt{\frac{2}{3}}K_{\alpha,\theta}\mathbf{n}\\ &\quad \left. + 2\langle\mu\rangle\Delta t\left[K_{,\theta}(\underline{1} - \underline{y}) : \underline{\dot{y}}\boldsymbol{\Sigma} + K(\underline{1} - \underline{y}) : \frac{\partial \underline{\dot{y}}}{\partial \theta}\boldsymbol{\Sigma} - E^{trip}_{\alpha}\hat{\mathbf{I}}_{dev} : \sqrt{\frac{2}{3}}H_{\alpha,\theta}\mathbf{n}\right]\right\}_{n+1} \quad (129)\end{aligned}$$

7.2 Coupling between temperature and inelastic energy dissipation

The matrix ${}^{t}_{0}\mathbf{K}_{\theta\theta}$ appearing in Eqs.(105) and (107) contains ${}^{t}_{0}\mathbf{K}^{\rho}$ which is the only undefined term in

Eq.(106).

The heat flux generated by dissipation of the inelastic strain energy contributes to the variation of the body stiffness, so that, the corresponding stiffness term has the form:

$$\mathbf{K}^{\rho} = \int_{V_0} \mathbf{H}^{\mathrm{T}} F_{\theta\,,\,\theta}^{in}\, dV_0. \tag{130}$$

and this belongs to the L.H.S of Eq.(98). This stiffness contribution is associated by the corresponding R.H.S. vector of Eq. (98)

$$\mathbf{F}^{\rho} = \int_{V_0} \mathbf{H}^{\mathrm{T}} F_{\theta\,,\,\theta}^{in}\, \theta^{(i-1)}\, dV_0 \tag{131}$$

where the derivative of the heat flux $F_{\theta}^{in} = f_{\theta}\left(\mathbf{T} : \dot{\mathbf{L}}^{in}\right)$ related to the dissipation of inelastic energy is

$$\frac{\partial F_{\theta}^{in}}{\partial \theta} \equiv F_{\theta\,,\theta}^{in} = f_{\theta}\left[\frac{\partial \mathbf{T}}{\partial \theta} : \dot{\mathbf{L}}^{in} + \frac{\partial \dot{\mathbf{L}}^{in}}{\partial \theta} : \mathbf{T}\right], \tag{132}$$

with $\mathbf{H}^{\mathrm{T}}$ as the finite element interpolation matrix. The derivative appeared in the second term of Eq.(132) is

$$\begin{aligned}\frac{\partial \dot{\mathbf{L}}^{in}}{\partial \theta} &= \frac{1}{\Delta t}\frac{\partial}{\partial \theta}\left[\bar{\Lambda}\mathbf{n} + \Delta t \dot{\mathbf{E}}^{trip}\right] \\ &= \frac{1}{\Delta t}\frac{\partial \bar{\Lambda}}{\partial \theta}\mathbf{n} + \frac{\partial \dot{\mathbf{E}}^{trip}}{\partial \theta}\end{aligned} \tag{133}$$

where $\frac{\partial \bar{\Lambda}}{\partial \theta}$ can be found by implicit differentiation of the yield function:

$$\begin{aligned}&\frac{\partial}{\partial \theta}\left[\gamma\|\boldsymbol{\Sigma}^*\| - 2\gamma\langle\mu\rangle\bar{\Lambda} - \gamma\sqrt{\frac{2}{3}}\Delta H_{\alpha} - \sqrt{\frac{2}{3}}K_{\alpha}\right] \\ = \;& \gamma_{,\theta}\|\boldsymbol{\Sigma}^*\| + 2\gamma\frac{\partial \boldsymbol{\Sigma}^*}{\partial \theta} : \boldsymbol{\Sigma}^* - 2\bar{\Lambda}\left\{\gamma_{,\theta}\langle\mu\rangle + \gamma\langle\mu\rangle_{,\theta}\right\} \\ & -2\gamma\langle\mu\rangle\frac{\partial \bar{\Lambda}}{\partial \theta} - \gamma_{,\theta}\sqrt{\frac{2}{3}}\Delta H_{\alpha} - \gamma\sqrt{\frac{2}{3}}H_{\alpha\,,\theta} \\ & -\sqrt{\frac{2}{3}}K_{\alpha\,,\theta}\end{aligned} \tag{134}$$

After re-ordering this can be expressed as

$$\begin{aligned}\frac{\partial \bar{\Lambda}}{\partial \theta} = \;& \frac{1}{2\gamma\langle\mu\rangle}\left[\gamma_{,\theta}\|\boldsymbol{\Sigma}^*\| + 2\gamma\frac{\partial \boldsymbol{\Sigma}^*}{\partial \theta} : \boldsymbol{\Sigma}^*\right. \\ & -2\bar{\Lambda}(\gamma_{,\theta}\langle\mu\rangle + \gamma\langle\mu\rangle_{,\theta})\gamma_{,\theta}\sqrt{\frac{2}{3}}\Delta H_{\alpha} \\ & \left. - -\gamma\sqrt{\frac{2}{3}}H_{\alpha\,,\theta} - \sqrt{\frac{2}{3}}K_{\alpha\,,\theta}\right]\end{aligned} \tag{135}$$

The other derivatives are defined as the following:

$$\begin{aligned}\gamma_{,\theta} \equiv \;& \frac{\partial \gamma}{\partial \theta} = \frac{\partial}{\partial \theta}\left[1 + 2\langle\mu\rangle\Delta t K(\underline{1} - \underline{y}) : \underline{\dot{y}}\right]^{-1} \\ = \;& -\left[1 + 2\langle\mu\rangle\Delta t K(\underline{1} - \underline{y}) : \underline{\dot{y}}\right]^{-2} \\ & 2\Delta t K\left[\langle\mu\rangle_{,\theta}(\underline{1} - \underline{y}) : \underline{\dot{y}} + \langle\mu\rangle(\underline{1} - \underline{y}) : \underline{\dot{y}}_{,\theta}\right]\end{aligned} \tag{136}$$

and

$$\begin{aligned}\frac{\partial \boldsymbol{\Sigma}^*}{\partial \theta} &= \frac{\partial}{\partial \theta}\left\{2\langle\mu\rangle\mathbf{I}_{dev} : \left[\Delta\mathbf{L} - \langle\alpha^{thm}\rangle\mathbf{1}\Delta\theta\right.\right. \\ & \left.\left. -\frac{1}{3}\Delta t\underline{\alpha}^{tra} : \underline{\dot{y}}\mathbf{1}\right]\right\} \\ &= 2\langle\mu\rangle_{,\theta}\mathbf{I}_{dev} : \left[\Delta\mathbf{L} - \frac{1}{3}\Delta t\underline{\alpha}^{tra} : \underline{\dot{y}}\mathbf{1}\right. \\ & \left. -\langle\alpha^{thm}\rangle\Delta\theta\mathbf{1}\right] + 2\langle\mu\rangle\mathbf{I}_{dev} : \\ & \left[-\left(\langle\alpha^{thm}\rangle_{,\theta}\Delta\theta + \langle\alpha^{thm}\rangle\right)\right. \\ & \left. -\frac{1}{3}\Delta t\left\{\underline{\alpha}_{,\theta}^{tra} : \underline{\dot{y}} + \underline{\alpha}^{tra} : \underline{\dot{y}}_{,\theta}\right\}\right]\mathbf{1}\end{aligned} \tag{137}$$

7.3 Temperature-displacement coupling

The stiffness matrix related to temperature-displacement coupling is defined by

$$\mathbf{K}_{\theta u} = \int_{V_0} \mathbf{H}^{\mathrm{T}}\frac{\partial F_{\theta}^{in}}{\partial \mathbf{L}}\mathbf{B}_L\, dV_0, \tag{138}$$

where the derivative of the corresponding heat flux generated by inelastic dissipation is

$$\frac{\partial F_{\theta}^{in}}{\partial \mathbf{L}} = f_{\theta}\left[\frac{\partial \mathbf{T}}{\partial \mathbf{L}} : \mathbf{L}^{in} + \frac{\partial \dot{\mathbf{L}}^{in}}{\partial \mathbf{L}} : \mathbf{T}\right]. \tag{139}$$

The derivative in the second term is derived from

$$\frac{\partial \dot{\mathbf{L}}^{in}}{\partial \mathbf{L}} = \frac{1}{\Delta t}\left[\frac{\partial \bar{\Lambda}}{\partial \mathbf{L}} \otimes \mathbf{n}\frac{\partial \Delta \mathbf{E}^{trip}}{\partial \mathbf{L}}\right], \tag{140}$$

with $\frac{\partial \Lambda}{\partial \mathbf{E}}$ given by Eq.(76), and $\frac{\partial \Delta \mathbf{E}^{trip}}{\partial \mathbf{L}}$ determined by Eq.(72).

7.4 Coupling between displacement and phase fractions

The finite element stiffness sub-matrix $\mathbf{K}_{uy}$ which couples displacement and phase fractions is defined by

$$\mathbf{K}_{uy} = \int_{V_0} \mathbf{B}_L^{\mathrm{T}}\mathbf{C}_{Ty}\, dV_0, \tag{141}$$

where

$$\mathbf{C}_{Ty} = \left[\; \left(\frac{\partial \mathbf{T}}{\partial \underline{y}}\right)_1 \;\; \left(\frac{\partial \mathbf{T}}{\partial \underline{y}}\right)_2 \;\; \cdots \;\; \left(\frac{\partial \mathbf{T}}{\partial \underline{y}}\right)_N \;\right]. \tag{142}$$

The coupling between a phase evolution and the stress requires also the definition of corresponding tangent modulus

$$\frac{\partial \mathbf{T}}{\partial \underline{y}}\bigg|_{n+1} =$$

$$\frac{\partial}{\partial \underline{y}}\Big\{\langle\kappa\rangle\left[\mathrm{tr}\Delta\mathbf{L} - \Delta t\underline{\alpha}^{tra} : \underline{\dot{y}} - \langle\alpha^{thm}\rangle\Delta\theta\right]\mathbf{1}$$
$$+\sqrt{\frac{2}{3}}\left(\Delta K_\alpha + \Delta H_\alpha\right)\mathbf{n} + 2\langle\mu\rangle\Delta t\dot{\mathbf{E}}^{TRIP}\Big\}$$
$$= \left[\mathbf{I} + 2\langle\mu\rangle\Delta t E_\alpha^{TRIP}\mathbf{I}_{dev}\right]^{-1} :$$
$$\Big\{\langle\kappa_{,\underline{y}}\rangle\left[\mathrm{tr}\Delta\mathbf{L} - \Delta t\underline{\alpha}^{tra} : \underline{y} - \langle\alpha^{thm}\rangle\Delta\theta\right]\mathbf{1}$$
$$+\langle\kappa\rangle\left[-\Delta t(\underline{\alpha}^{tra}_{,\underline{y}} : \underline{\dot{y}} + \alpha^{tra} : \underline{\dot{y}}_{,\underline{y}}) - \langle\alpha^{thm}_{,\underline{y}}\rangle\Delta\theta\right]\mathbf{1}$$
$$\sqrt{\frac{2}{3}}\left(K_{\alpha,\underline{y}} + H_{\alpha,\underline{y}}\right)\otimes\mathbf{n} + \frac{2}{3}(K'_\alpha + H'_\alpha)\frac{\partial\bar{\Lambda}}{\partial \underline{y}}\otimes\mathbf{n}$$
$$+2\langle\mu\rangle_{,\underline{y}}\Delta t\mathbf{E}^{TRIP} + 2\langle\mu\rangle\Delta t\frac{\partial E_\alpha^{TRIP}}{\partial \underline{y}}\otimes\mathbf{\Sigma}\Big\} \tag{143}$$

and

$$\frac{\partial E_\alpha^{TRIP}}{\partial \underline{y}} = \underline{\dot{y}}_{,\underline{y}} : (\underline{1} - \underline{y}) - \underline{I} : \underline{\dot{y}} \tag{144}$$

where the identity matrix for the phase-fraction vector is:

$$\underline{I} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ & & \ddots & & \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}$$

which size depends on a number of considered phases.

7.5 Coupling between temperature and phase fraction

The contribution to the global stiffness matrix arising from the coupling of temperature and phase transformations is defined by

$$\mathbf{K}_{\theta y} = \int_{V_0} \mathbf{H}^{\mathrm{T}}\frac{\partial F_\theta^{in}}{\partial \underline{y}}\,dV_0, \tag{145}$$

with the corresponding heat flux derivative expressed by

$$\frac{\partial F_\theta^{in}}{\partial \underline{y}} = f_\theta\left[\frac{\partial \mathbf{T}}{\partial \underline{y}} : \dot{\mathbf{L}}^{in} + \frac{\partial \dot{\mathbf{L}}^{in}}{\partial \underline{y}} : \mathbf{T}\right]. \tag{146}$$

The derivative in the second term of the R.H.S. is written as

$$\frac{\partial \dot{\mathbf{L}}^{in}}{\partial \underline{y}} = \frac{1}{\Delta t}\frac{\partial}{\partial \underline{y}}\left[\bar{\Lambda}\mathbf{n} + \Delta t\dot{\mathbf{E}}^{trip}\right] = \frac{1}{\Delta t}\frac{\partial\bar{\Lambda}}{\partial \underline{y}}\mathbf{n} + \frac{\partial\dot{\mathbf{E}}^{trip}}{\partial \underline{y}}. \tag{147}$$

The derivative $\frac{\partial\bar{\Lambda}}{\partial \underline{y}}$ can be found by implicit differentiation of the consistency condition

$$\frac{\partial}{\partial \underline{y}}\left[\gamma\|\mathbf{\Sigma}^*\| - 2\gamma\langle\mu\rangle\bar{\Lambda} - \gamma\sqrt{\frac{2}{3}}\Delta H_\alpha - \sqrt{\frac{2}{3}}K_\alpha\right] =$$
$$\gamma_{,\underline{y}}\|\mathbf{\Sigma}^*\| + 2\gamma\frac{\partial\mathbf{\Sigma}^*}{\partial \underline{y}} : \mathbf{\Sigma}^* - 2\bar{\Lambda}\left[\gamma_{,\underline{y}}\langle\mu\rangle + \gamma\langle\mu\rangle_{,\underline{y}}\right]$$
$$-2\gamma\langle\mu\rangle\frac{\partial\bar{\Lambda}}{\partial \underline{y}} - \gamma_{,\underline{y}}\sqrt{\frac{2}{3}}\Delta H_\alpha - \gamma\sqrt{\frac{2}{3}}H_{\alpha,\underline{y}}$$
$$-\sqrt{\frac{2}{3}}K_{\alpha,\underline{y}} = 0, \tag{148}$$

and taking $\frac{\partial\bar{\Lambda}}{\partial \underline{y}}$ to the L.H.S.

$$\frac{\partial\bar{\Lambda}}{\partial \underline{y}} = \frac{1}{2\gamma\langle\mu\rangle}\Big[\gamma_{,\underline{y}}\|\mathbf{\Sigma}^*\| + 2\gamma\frac{\partial\mathbf{\Sigma}^*}{\partial \underline{y}} : \mathbf{\Sigma}^*$$
$$-2\bar{\Lambda}(\gamma_{,\underline{y}}\langle\mu\rangle + \gamma\langle\mu\rangle_{,\underline{y}})$$
$$-\gamma_{,\underline{y}}\sqrt{\frac{2}{3}}\Delta H_\alpha - \gamma\sqrt{\frac{2}{3}}H_{\alpha,\underline{y}} - \sqrt{\frac{2}{3}}K_{\alpha,\underline{y}}\Big] \tag{149}$$

The other derivatives in Eq.(149) are given by

$$\gamma_{,\underline{y}} = \frac{\partial}{\partial \underline{y}}\left[1 + 2\langle\mu\rangle\Delta t K(\underline{1} - \underline{y}) : \underline{\dot{y}}\right]^{-1}$$
$$= -\left[1 + 2\langle\mu\rangle\Delta t K(\underline{1} - \underline{y}) : \underline{\dot{y}}\right]^{-2}$$
$$2\Delta t K\Big[\langle\mu\rangle_{,\underline{y}}(\underline{1} - \underline{y}) : \underline{\dot{y}}$$
$$+\langle\mu\rangle\left\{(\underline{1} - \underline{y}) : \underline{\dot{y}}_{,\underline{y}} - \underline{I} : \underline{\dot{y}}\right\}\Big], \tag{150}$$

$$\frac{\partial\mathbf{\Sigma}^*}{\partial \underline{y}} = \frac{\partial}{\partial \underline{y}}\Big\{2\langle\mu\rangle\mathbf{I}_{dev} : \Big[\Delta\mathbf{L} - \langle\alpha^{thm}\rangle\mathbf{1}\Delta\theta$$
$$-\frac{1}{3}\Delta t\underline{\alpha}^{tra} : \underline{\dot{y}}\mathbf{1}\Big]\Big\}$$
$$= 2\langle\mu\rangle_{,\underline{y}}\mathbf{I}_{dev} : \Big[\Delta\mathbf{L} - \frac{1}{3}\Delta t\underline{\alpha}^{tra} : \underline{\dot{y}}\mathbf{1}$$
$$-\langle\alpha^{thm}\rangle\Delta\theta\mathbf{1}\Big]$$
$$+2\langle\mu\rangle\mathbf{I}_{dev} : \Big[-\left\{\langle\alpha^{thm}\rangle_{,\underline{y}}\Delta\theta + \langle\alpha^{thm}\rangle\right\}$$
$$-\frac{1}{3}\Delta t\left\{\underline{\alpha}^{tra}_{,\underline{y}} : \underline{\dot{y}} + \underline{\alpha}^{tra} : \underline{\dot{y}}_{,\underline{y}}\right\}\Big]\mathbf{1}. \tag{151}$$

The derivative in the second term of Eq.(147) is expressed by

$$\frac{\partial\dot{\mathbf{E}}^{trip}}{\partial \underline{y}} = \frac{\partial}{\partial \underline{y}}\left[K(\underline{1} - \underline{y}) : \underline{\dot{y}}\right]\mathbf{\Sigma}$$
$$= K\left[(\underline{1} - \underline{y}) : \underline{\dot{y}}_{,\underline{y}} - \underline{I} : \underline{\dot{y}}\right]\mathbf{\Sigma} + K(\underline{1} - \underline{y}) : \underline{\dot{y}}\frac{\partial\mathbf{\Sigma}}{\partial \underline{y}}$$
$$= K\left[(\underline{1} - \underline{y}) : \underline{\dot{y}}_{,\underline{y}} - \underline{I} : \underline{\dot{y}}\right]\mathbf{\Sigma} + K(\underline{1} - \underline{y}) : \underline{\dot{y}}$$
$$\left[\left(\hat{\mathbf{I}}_{dev} : \frac{\partial\mathbf{T}}{\partial \underline{y}}\right) - \sqrt{\frac{2}{3}}H'_\alpha\frac{\partial\bar{\Lambda}}{\partial \underline{y}}\mathbf{n}\right] \tag{152}$$

8. Matrices of FE Phase Evolution Equation

8.1 Ferritic and Pearlitic Transformations

The general form of evolution law for ferritic and pearlitic diffusional transformations, that has been proposed in [20], can be written in the following form:

$$\begin{aligned}\dot{y}_i^\phi &= \mathcal{A}_i\left(\mathbf{S},\theta,y_i^\phi,t\right)\dot{\theta}+\mathcal{B}_i\left(\mathbf{S},\theta,y_i^\phi,t\right)\dot{\mathbf{S}} \\ &+\mathcal{R}_i\left(\mathbf{S},\theta,y_i^\phi,t\right),\end{aligned} \tag{153}$$

where $\dot{y}_i^\phi$ is the fictitious ferrite or pearlite phase fraction, $\mathcal{A}_i$, $\mathcal{B}_i$, and $\mathcal{R}_i$ are material functions, and subscript i assumes one of two values: 2 or 3. The time approximation and linearization leads to the linear expression

$${}^{t+\Delta t}\dot{\mathbf{y}}_i^\phi = {}^t\mathcal{A}_i\ {}^{t+\Delta t}\dot{\theta}+{}^t\mathcal{B}_i\ {}^{t+\Delta t}_{\ 0}\dot{\mathbf{S}}+{}^t\mathcal{R}_i. \tag{154}$$

The rate of the second Piola-Kirchhoff stress must be transformed to the increment of displacement $\Delta\mathbf{u}$ before this equation will be substituted to the global FE equation for thermo-mechanical-metallurgical problem. Such transformation can be derived using elastic constitutive equation and strain-displacement matrices. The evolution equation expressed in terms of temperature rate and displacement increment can be written as

$${}^{t+\Delta t}\dot{\mathbf{y}}_i^\phi = {}^t\mathcal{A}_i\ {}^{t+\Delta t}\dot{\theta}+{}^t\hat{\mathcal{B}}_i\ {}^{t+\Delta t}\dot{\mathbf{u}}+{}^t\hat{\mathcal{R}}_i. \tag{155}$$

where particular forms of ${}^t\hat{\mathcal{B}}_i$ and ${}^t\hat{\mathcal{R}}_i$ will be shown after introducing constitutive equations for elastic and inelastic deformations.

The simplest evolution equation for diffusional transformations, without metallurgical- mechanical coupling, is given by

$$\dot{y}_i^\phi = \left(1-y_i^\phi\right)\left[\frac{db_i}{d\theta}\dot{\theta}+\frac{b_i(\theta)n_i}{t}\right]t^{n_i}, \tag{156}$$

which after time approximation can be written as the following:

$${}^{t+\Delta t}\dot{\mathbf{y}}_i^\phi = {}^t\mathcal{A}\ {}^{t+\Delta t}\dot{\theta}+{}^t\mathcal{R}, \tag{157}$$

with factors given by

$$\begin{aligned}{}^t\mathcal{A} &= \left(1-{}^t\mathbf{y}_i^\phi\right){}^t t^{n_i}\left[\frac{db_i}{d\theta}\right]_t; \\ {}^t\mathcal{R} &= \left(1-{}^t\mathbf{y}_i^\phi\right){}^t t^{n_i-1}\ {}^t b_i\ n_i,\end{aligned} \tag{158}$$

where b_i and n_i are empirical related to cooling rate and the nucleation rate, t is time equal to zero at the nucleation period.

8.2 Bainitic Transformation

The evolution equation for bainitic transformation, shown in [20], can be written in the following form:

$$\begin{aligned}\dot{y}_4^\phi &= \frac{V^{mic}K_1}{\gamma}\left(1-y_4^\phi\right)\left(1-\beta\gamma y_4^\phi\right)\times \\ &\exp\left[\langle\Gamma_2\rangle y_4^\phi-\frac{K_2}{R\theta}\left(1-\frac{\langle\Delta G^0_{4_{max}}\rangle}{r}\right)\right],\end{aligned} \tag{159}$$

$$\langle\Gamma_2\rangle = \frac{K_2\langle\Delta G^0_{4_{max}}-G_N\rangle}{r\,R\,\theta} \tag{160}$$

where V^{mic} is the volume of a microregion, K_1 is the parameter related to austenite grain size, $\gamma = y_\gamma\ y_{4_{max}}$, y_γ is the fraction of residual austenite, β is the autocatalysis factor, K_2 is constant, R is gas constant, $\Delta G^0_{4_{max}}$ is the change of maximum nucleation free energy determined from the free energy diagram, r is the positive constant appearing in approximation of the value G_N that is exceeded by $\Delta G^0_{4_{max}}$ at temperature W_s. Note that this equation does not contain rates of variables controlling bainitic transformation. The time approximation and linearization results in the relationship

$$\begin{aligned}{}^{t+\Delta t}\dot{\mathbf{y}}_4^\phi &= \left(1-{}^t\mathbf{y}_4^\phi\right)\left(1-A_1\ {}^t\mathbf{y}_4^\phi\right)A_2 \\ &\times\exp\left[\frac{A_3}{{}^t\theta}\left({}^tG_1\ {}^t\mathbf{y}_4^\phi-{}^tG_2\right)\right]\end{aligned} \tag{161}$$

where

$$\begin{aligned}A_1 &= \beta\gamma;\ A_2=\frac{V^{mic}K_1}{\gamma};\ A_3=\frac{K_2}{r\,R}; \\ {}^tG_1 &= \left[\langle\Delta G^0_{4_{max}}-G_N\rangle\right]_t; \\ {}^tG_2 &= r-\left[\langle\Delta G^0_{4_{max}}\rangle\right]_t.\end{aligned}$$

The general form of Eq.(161) can be expressed by

$${}^{t+\Delta t}\dot{\mathbf{y}}_4^\phi = {}^t\mathcal{A}_4\exp\left(\frac{{}^t\mathcal{F}}{{}^t\theta}\right), \tag{162}$$

where

$$\begin{aligned}{}^t\mathcal{A}_4 &\equiv \left(1-{}^t\mathbf{y}_4^\phi\right)\left(1-A_1\ {}^t\mathbf{y}_4^\phi\right)A_2; \\ {}^t\mathcal{F} &\equiv A_3\left({}^tG_1\ {}^t\mathbf{y}_4^\phi-{}^tG_2\right).\end{aligned}$$

8.3 Martensitic Transformation

The general form of evolution equation for martensitic transformation shown in [20] following the proposition [9], can be written as the following kinetic law:

$$\dot{y}_6 = \mathcal{A}_6\left(\mathbf{S},\theta,\hat{y}_6,t\right)\dot{\theta}+\mathcal{K}_6\left(\mathbf{S},\theta,\hat{y}_6,t\right)\mathbf{E}^*_{cr}:\dot{\mathbf{S}}, \tag{163}$$

where $\mathcal{A}_6$ and $\mathcal{K}_6$ are material functions, $\mathbf{E}^*_{cr}$ is a value of the macroscopic transformation strain $\mathbf{E}^*$ when $y_6=1$ and stress $\mathbf{S}$ is assumed to be homogeneous in a microregion representing a group of finite elements.

This stress is balancing the external stress load. The time approximation and linearization result in the expression

$$^{t+\Delta t}\dot{\hat{\mathbf{y}}}_6 = {}^t\mathcal{A}_6 \; {}^{t+\Delta t}\dot{\theta} + {}^t\mathcal{B}_6 \; {}^{t+\Delta t}_{0}\dot{\mathbf{S}}, \quad (164)$$

with

$$^t\mathcal{B}_6 = {}^t\mathcal{K}\,\mathbf{E}^*_{cr}. \quad (165)$$

Transformation of stress $^{t+\Delta t}_{0}\dot{\mathbf{S}}$ to strain rate $\dot{\mathbf{E}}$ and velocity $\dot{\mathbf{u}}$ leads to the following martensitic growth law

$$^{t+\Delta t}\dot{\hat{\mathbf{y}}}_6 = {}^t\mathcal{A}_6 \; {}^{t+\Delta t}\dot{\theta} + {}^t\hat{\mathcal{B}}_6 \; {}^{t+\Delta t}\dot{\mathbf{u}} + {}^t\hat{\mathcal{R}}_6, \quad (166)$$

where $^t\hat{\mathcal{B}}_6$ and $^t\hat{\mathcal{R}}_6$ will be derived later using elastic constitutive equations.

The simplest evolution equation for martensitic fraction is given by

$$\dot{\hat{y}}_6 = \alpha\,(1 - \hat{y}_6)\,\dot{\theta}, \quad (167)$$

which after time approximation can be re-written as the following

$$^{t+\Delta t}\dot{\hat{\mathbf{y}}}_6 = {}^t\mathcal{A}_6 \; {}^{t+\Delta t}\dot{\theta}, \quad (168)$$
$$^t\mathcal{A}_6 = \alpha\left(1 - {}^t\hat{\mathbf{y}}_6\right),$$

where α is the constant coefficient that for most steels equals to $1.1 \times 10^{-2}[K^{-1}]$.

Matrices $^t\mathcal{B}_i$, $^t\hat{\mathcal{B}}_6$, $^t\hat{\mathcal{R}}_i$, and $^t\hat{\mathcal{R}}_6$ in Eqs.(155) and (166) are derived using elastic constitutive relation Eq.(44) expressed in the form:

$$^{t+\Delta t}_{0}\dot{\mathbf{S}}^{(i)} = 2\mu\left({}^{t+\Delta t}_{0}\dot{\mathbf{E}}^{\Delta(i)} - {}^{t+\Delta t}_{0\,in}\dot{\mathbf{E}}^{\Delta(i-1)}\right)$$
$$+\frac{\dot{\mu}}{\mu}\,{}^t_0\mathbf{S}, \quad (169)$$

where $^{t+\Delta t}_{0\,in}\dot{\mathbf{E}}^{\Delta(i-1)}$ is the inelastic strain rate defined for the previous iteration $(i-1)$. Substituting the following relation:

$$^{t+\Delta t}_{0}\dot{\mathbf{E}}^{\Delta(i)} = \left({}^t_0\mathbf{B}_L + {}^t_0\mathbf{B}^{\mathrm{T}}_{nL}\,{}^t_0\mathbf{B}_{nL}\right)\,{}^{t+\Delta t}\dot{\mathbf{u}} \quad (170)$$

to Eq.(169) results in the equation

$$^{t+\Delta t}_{0}\dot{\mathbf{S}}^{(i)} = \breve{\mathcal{B}}\;{}^{t+\Delta t}\dot{\mathbf{u}} - {}^{t+\Delta t}\breve{\mathcal{R}} + {}^t\breve{\mathcal{R}} \quad (171)$$
$$\breve{\mathcal{B}} = 2\mu\left({}^t_0\mathbf{B}_L + {}^t_0\mathbf{B}^{\mathrm{T}}_{nL}\,{}^t_0\mathbf{B}_{nL}\right);$$
$$^{t+\Delta t}\breve{\mathcal{R}} = 2\mu\;{}^{t+\Delta t}_{0\,\mathbf{in}}\dot{\mathbf{E}}^{\Delta(i-1)};$$
$$^t\breve{\mathcal{R}} = \frac{\dot{\mu}}{\mu}\,{}^t_0\mathbf{S}.$$

Combining Eq.(171) with Eq.(154) leads to the form of the evolution law for ferritic-pearlitic transformation

$$^{t+\Delta t}\dot{\mathbf{y}}^{\phi}_i = {}^t\mathcal{A}_i\;{}^{t+\Delta t}\dot{\theta} + {}^t\mathcal{B}_i\,\breve{\mathcal{B}}\;{}^{t+\Delta t}\dot{\mathbf{u}}$$
$$-{}^t\mathcal{B}_i\;{}^{t+\Delta t}\breve{\mathcal{R}} + {}^t\mathcal{B}_i\;{}^t\breve{\mathcal{R}} + {}^t\mathcal{R}_i. \quad (172)$$

Introducing the following symbols:

$$^t\hat{\mathcal{B}} = {}^t\mathcal{B}_i\,\breve{\mathcal{B}};$$
$$^t\hat{\mathcal{R}}_i = {}^t\mathcal{B}_i\;{}^t\breve{\mathcal{R}} + {}^t\mathcal{R}_i - {}^t\mathcal{B}_i\;{}^{t+\Delta t}\breve{\mathcal{R}} \quad (173)$$

into Eq.172 results in the Eq.(155). Substituting Eq.(171) in Eq.(164) gives

$$^{t+\Delta t}\dot{\hat{\mathbf{y}}}_6 = {}^t\mathcal{A}_6\;{}^{t+\Delta t}\dot{\theta} + {}^t\mathcal{B}_6\,\breve{\mathcal{B}}\;{}^{t+\Delta t}\dot{\mathbf{u}}$$
$$+{}^t\mathcal{B}_6\;{}^t\breve{\mathcal{R}} - {}^t\mathcal{B}_6\;{}^{t+\Delta t}\breve{\mathcal{R}}. \quad (174)$$

Denoting

$$^t\hat{\mathcal{B}}_6 = {}^t\mathcal{B}_6\,\breve{\mathcal{B}};$$
$$^t\hat{\mathcal{R}}_6 = {}^t\mathcal{B}_6\left({}^t\breve{\mathcal{R}} - {}^{t+\Delta t}\breve{\mathcal{R}}\right). \quad (175)$$

results in Eq.(166).

9. Conclusions

The structure of FE program developed for solution of TMM problem is shown in **Fig. 3**. Constitutive equations for macroregions are coupled with heat equation and evolution laws by the mixture rule. This scheme facilitates transformation of micro-structural state variables: phase fractions, isobaric macroregional stresses, cooling and nucleation rates, the Gibbs free energy changes, etc. to the level of global state variables for considered body. Constraints for this transformation are the mixture rule and the balance of virtual work for isobaric macro-elements. The microstructure of alloy is approximated by super-elements, which corresponds to grains. Each super-element is composed of several ordinary finite elements that contain various microregions or phases represented at Gaussian nodes of integration. This hierarchy in approximation of material properties provides a transmission of micro-material state variables to the macrolevel of finite element method solution of welding problem.

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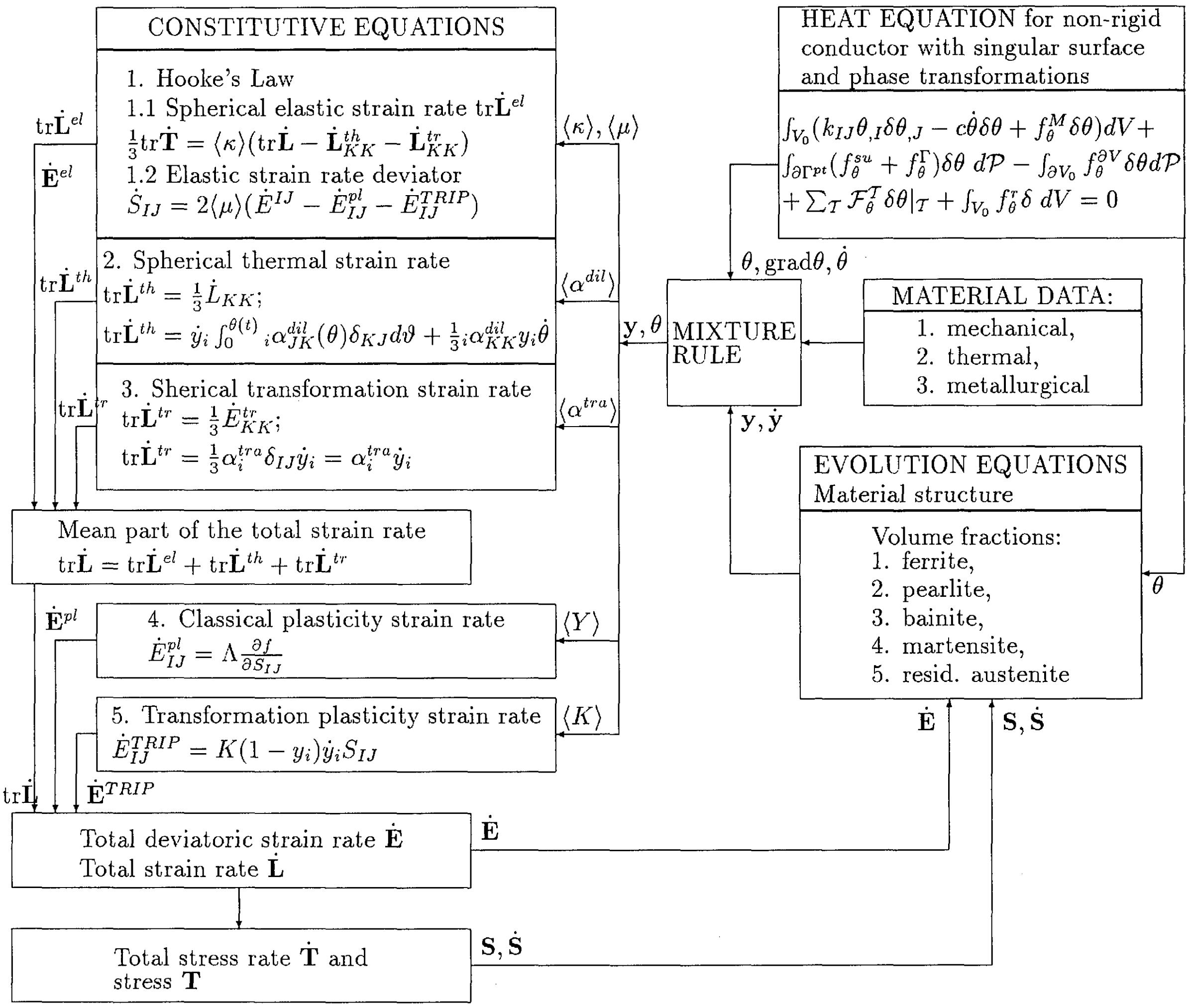

Fig 3 Scheme for solution of TMM problem

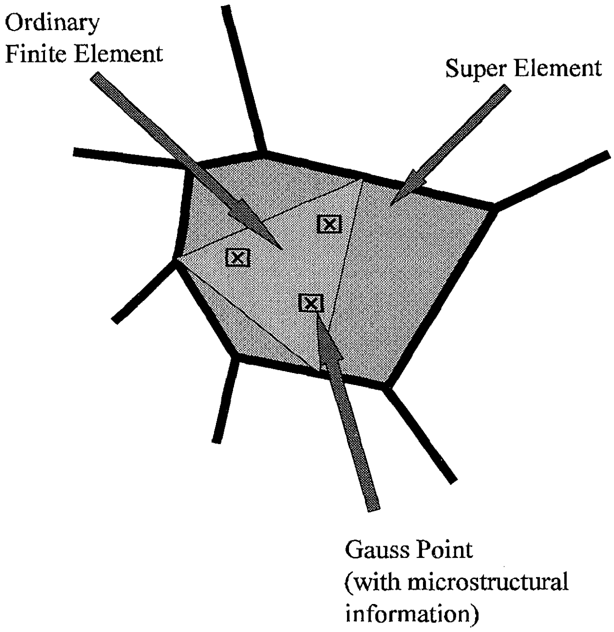

Fig 4 Finite element microstructure approximation hierachy

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