MACRO-, MESO- AND MICRO-SCOPIC METALLO-THERMO-MECHANICS
--- Theories and applications ---

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Coupling among metallic structures including molten state, temperature, and stress and/or strain occurring in processes accompanied by phase transformation sometimes affects predominant influence in determining such fields in industrial processes as quenching, welding, casting and so on. Outer triangle in figure 1 represents the schematic representation of the effect of *metallo-thermo-mechanical coupling* with the induced phenomena. When the temperature distribution in a material varies, *thermal stress* is caused in the body, and the induced phase transformation affects the structural distribution, which is well known during melting or solidification in solid-liquid transition and austenite-pearlite or -martensite transformation in solid phase. Local dilatation due to structural changes in the body bring out the *transformation stress* and interrupts the stress or strain field in the body, and effect of transformation plasticity on the stress/strain constitutive equation is not also negligible.

In contrast to these phenomena, which are well known in ordinal analysis, arrows in the opposite direction indicate coupling in the following manner. Part of the *mechanical work* done by the existing stress in the material is converted into heat, which may be predominant in the case of inelastic deformation, thus disturbing the temperature distribution. The acceleration of phase transformation by stress or strain, which is called *stress- or strain-induced transformation*, has been treated by metallurgists as one of leading parameters of transformation kinetics. The opposite arrow corresponds to the *latent heat* due to phase transformation, which is essential in determining the temperature. When no coupling among the fields, independent analyses of heat conduction, stress and transformation kinetics are possible to be carried out. However, in such case of coupled issue, global formulation based on continuum thermodynamics is needed.

Formulation of the fundamental coupled equations for stress-strain relationships, heat conduction and transformation kinetics based on continuum thermodynamics will be made in the first part of this paper, and the finite element implementation is carried out, which is termed as ***macroscopic metallo-****thermo-mechanics* (or, in general, *materio-thermo-mechanics*).

However, if we treat the motion of atoms or molecules consisting of the continuum, all three fields are identified by solving Newton equations of motion for each atom, since the structural change depends on the *configuration*, temperature is the *vibration* itself and stress/strain is related to the *interatomic distance* as is shown by the inner illustration in the figure. *Molecular dynamics method* is one of the most promising techniques to emit a light especially to such kind of coupled metallo-thermo-mechanical problems. The way to solve the problem is here called ***microscopic, or nanoscopic metallo-thermo-mechanical approach.***

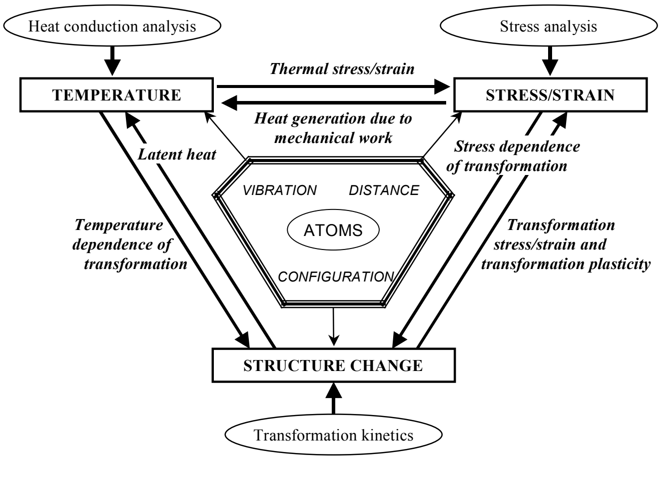

Figure 1. Macro- and micro-scopic representation of *metallo-thermo-mechanics.*

In such a situation of the restriction of so small domain and so short time period to be treated by the molecular dynamics simulation, the *phase field method* has been developed as a promising technique to solve the fields of phase change associated with temperature, and some successful results are obtained for initiation and growth of solidifying crystal from liquid state, and in-solid phase transformation. However, few papers for the phase field method treat the mechanical field of stress and strain.

In the first half of this paper, thermodynamic consideration will be presented to derive the series of fundamental equations governing the coupled mechanical, thermal and phase fields, which the author calls as a ***mesoscopic metallo-thermo-mechanics***.

A parameter ψ termed as *transformation parameter* representing the structural change due to in-solid or solid-liquid transformation is introduced, which will be reduced to a volume fraction ξ in the former case and a phase field parameter ϕ in the latter case. Based on the continuum thermodynamics, the evolution equation of the parameter is obtained from the restriction of continuum thermodynamics ;

$$\tau\dot{\psi} = TK(\psi) - \frac{\partial G}{\partial \psi}$$

with a positive constant τ, and free energy function G as well as the coupled heat conduction equation and stress-strain constitutive equation.

$$\rho c\dot{T} = \sigma_{ij}\dot{\varepsilon}_{ij} - \frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right) + \rho\gamma + K_u(\psi)\dot{\psi}$$

$$\varepsilon_{ij}^{\mathrm{e}} = \left(\Sigma\frac{1+\nu_I}{E_I}\xi_I\right)\sigma_{ij} - \left(\Sigma\frac{\nu_I}{E_I}\xi_I\right)\delta_{ij}\sigma_{kk} + \delta_{ij}\int_{T_0}^{T}\Sigma\alpha_I\xi_I dT + \delta_{ij}\Sigma\beta_I(\xi_I - \xi_{I0})$$

Applications of the derived equations are now introduced to solve some engineering processes incorporating phase transformation, such as quenching of a gear wheel and a sword by the finite element method as the macroscopic application and dendrite growth coupled with mechanical field by the phase field method as mesoscopic viewpoint. Some results on melting and /or solidification depending on stress by the molecular dynamics method are also presented as example of microscopic simulation.