

On the Coupling of Mass Diffusion and Non-Mechanical Energy Flow in Metals under Finite Deformation

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Abstract: The governing equation of non-mechanical energy flow in metals, undergoing finite deformation, is presented. The coupling of non-mechanical energy flow, mass diffusion and metal elastic-plastic deformation is rigorously taken into account. The analysis is particularly useful in cases of diffusion-driven degradation mechanisms ahead of stationary cracks or cracks initiating growth, under temperature variations.

INTRODUCTION

If an initially homogeneous single-phase iron-carbon alloy is held at a constant temperature gradient, carbon diffuses up the temperature gradient, leading to an increase of carbon concentration at the hot end (e.g. [1] for 0.01% C). On the other hand, if a zirconium-based alloy, with an initially homogeneous distribution of hydrogen, is subjected to a temperature gradient, hydrogen moves towards the cold end (e.g. [2]). Both are thermal transport phenomena, indicating the coupling of mass diffusion and heat conduction. There are several experimental studies of thermal transport of mass in metals, for example of hydrogen, deuterium and carbon in bcc α -Fe and V, in fcc Ni, Co and Pd and in hcp Zr (e.g. [1], [3]).

Coupled processes of mass diffusion and heat conduction in metals have important industrial implications. In chemical and petro-chemical industry hydrogen-induced degradation processes in steel structures may occur. In the case of hydrogen attack, at high temperatures and hydrogen pressures, hydrogen diffuses in steel and reacts with carbides forming methane. Due to its large molecule size, methane is trapped and forms voids, which grow and eventually lead to material failure. Hydrogen embrittlement of steel is another severe type of material degradation, which can cause failure under very low loads, compared to those sustained by a hydrogen-free material. The physical process is not clear. Several mechanisms have been proposed: hydrogen enhanced decohesion, hydrogen enhanced localized plasticity, adsorption-induced localized slip and hydrogen pressurization. However, an important and undisputed part of the physical process involves the diffusion of hydrogen towards the site of material degradation. Similar phenomena of hydrogen embrittlement occur in other metals, such as nickel and aluminum. In hydride forming metals, such as niobium, vanadium and zirconium, the embrittlement mechanism has been well understood. In this case, the degradation of the material is caused by the brittle hydrides, which precipitate in places, where the concentration of hydrogen is sufficiently high. Again an important part of the degradation process involves

the diffusion of hydrogen towards the sites of hydride formation.

Precise mathematical models [3-5] for the simulation of hydride-induced embrittlement and fracture in metals have been developed in recent years. These models take into account the coupling of the operating physical processes, namely: (i) hydrogen diffusion, (ii) hydride precipitation, (iii) non-mechanical energy flow (i.e. flow of heat and energy carried by the diffusing mass) and (iv) hydride/solid-solution deformation. These models are general and therefore they are applicable to other degradation phenomena, which involve mass diffusion and heat conduction. They are based on infinitesimal displacement gradient theory. In the case of steady-state crack growth, the deformation of the material is adequately described by infinitesimal displacement gradient theory [6] (see also [7] and referenced publications). However, in the case of stationary cracks or during initial crack growth, infinitesimal displacement gradient theory is sufficient only outside the region of crack tip blunting. Thus, these models can be further improved by considering metal finite deformation near the blunted crack tip.

A limited number of simulations of hydrogen embrittlement in metals, under finite deformation, have been performed, which take into account the coupling of hydrogen diffusion, elastic-plastic material deformation (e.g. [8-10]) and hydride precipitation (e.g. [11-12]). Non-mechanical energy flow is not considered in these simulations. However, the models, which are used in the above-mentioned simulations, need to be modified in order to employ the correct form of the governing equation of mass diffusion under finite deformation, derived in [7].

In the present study, the governing equations for the coupled processes of mass diffusion and non-mechanical energy flow in a metal under finite deformation are discussed. Therefore the present letter provides the information, which is required for investigating mass diffusion and non-mechanical energy flow near a blunted crack tip. Thus the improvement of the existing mathematical models for the simulation of coupled mass-diffusion / heat-conduction degradation processes is facilitated.

In the following, tensor notation is used throughout. Bold-faced symbols are used to denote vectors and second-

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order tensors. Products are indicated with dots and products containing no dots are dyadic products. Latin indices range from one to three and repeated Latin indices are always summed. Inverses, transposes and transposed inverses are denoted with a superscripted -1 , T and $-T$, respectively. For example:

$$\mathbf{A} \cdot \mathbf{B} = A_{ik} B_{kj} \mathbf{b}_i \mathbf{b}_j ,$$

$$\mathbf{A} : \mathbf{B} = A_{ij} B_{ji} ,$$

$$\mathbf{c} \mathbf{d} = c_i d_j \mathbf{b}_i \mathbf{b}_j ,$$

$$\mathbf{c} \cdot \mathbf{d} = c_i d_i ,$$

$$\mathbf{B} \cdot \mathbf{c} = B_{ik} c_k \mathbf{b}_i .$$

The base vectors, \mathbf{b}_i , are Cartesian and independent of time, t .

GOVERNING EQUATIONS OF MASS DIFFUSION AND NON-MECHANICAL ENERGY FLOW

The body of a metallic solid is subjected to externally applied loads and undergoes elastic-plastic finite deformation, described by the deformation gradient \mathbf{F} ($= \partial \mathbf{x} / \partial \mathbf{X}$); \mathbf{x} is the position of a solid particle in the deformed configuration at time t (spatial coordinates) and \mathbf{X} is its position in a reference (non-deformed) configuration (material coordinates). The rate of deformation, \mathbf{D} , is given by the following well-known relation:

$$\mathbf{D} = \text{sym} \left(\frac{d\mathbf{F}}{dt} \cdot \mathbf{F}^{-1} \right) , \quad (1)$$

where *sym* denotes the symmetric part of a tensor. The deformation gradient is decomposed into elastic and plastic parts [13]:

$$\mathbf{F} = \partial \mathbf{x} / \partial \mathbf{X} = \mathbf{F}^* \cdot \mathbf{F}^p . \quad (2)$$

\mathbf{F}^p is the deformation gradient due solely to the plastic flow. \mathbf{F}^* is the remaining contribution to \mathbf{F} , associated with the elastic distortion, any rigid rotation and any stress-free expansion of the material. The configuration, which is obtained by applying the mapping \mathbf{F}^p to the reference configuration, is the intermediate configuration. The multiplicative decomposition of the deformation gradient, described by (2), has been used successfully in several applications. For example, it has been used in applications of crystal plasticity [14], elastic-plastic fracture mechanics [15] and dynamic plastic flow [16]. The multiplicative decomposition is the natural composition law for successive finite motions and contains all the necessary information for the measurement of plastic strains and the computation of anelastic power. The interested reader is also referred to the discussion, by Maugin [17], on the decomposition of finite strains, existing models, and the advantages of multiplicative decomposition.

The elastic response of the solid is described on the intermediate configuration (e.g. [18]), where the Lagrangian strain, \mathbf{E}^* , and the second Piola-Kirchhoff stress, \mathbf{S}^* , are defined as follows:

$$\mathbf{E}^* = (1/2) (\mathbf{F}^{*T} \cdot \mathbf{F}^* - \mathbf{I}) , \quad (3a)$$

$$\mathbf{S}^* = \mathbf{F}^{*-1} \cdot \boldsymbol{\tau} \cdot \mathbf{F}^{*-T} . \quad (3b)$$

$\boldsymbol{\tau} = |\mathbf{F}| \boldsymbol{\sigma}$ is Kirchhoff stress, $|\mathbf{F}|$ is the determinant of the deformation gradient and $\boldsymbol{\sigma}$ is Cauchy stress. Cauchy stress is defined on the deformed, by \mathbf{F} , configuration. Also \mathbf{I} is the second order identity tensor.

The solid contains a diffusing substance, which has a concentration (e.g. number of moles per unit volume) in the deformed configuration given by c^M ; the superscript M is used to denote the diffusing substance. The dissolution of the substance in the solid generally causes a stress-free expansion, contributing to \mathbf{F}^* . The conservation of the mass of the diffusing substance is given by the following relation, originally derived by the author in the case of a solid, undergoing finite deformation [7]:

$$\frac{dc^M}{dt} + c^M \nabla \cdot \mathbf{v} + \nabla \cdot \mathbf{j}^M = 0 . \quad (4)$$

d/dt is material time derivative, taken at a specified solid particle in the reference configuration. Material time derivative, on the deformed configuration, satisfies the relation: $d/dt = \partial/\partial t + \mathbf{v} \cdot \nabla$, where $\partial/\partial t = (\partial/\partial t)_x$ is the partial time derivative, related to a point in space and not to a solid particle in the reference configuration, and $\nabla = \mathbf{b}_k \partial/\partial x_k$. \mathbf{v} is the velocity of a solid particle. \mathbf{j}^M is the flux of the diffusing substance, which in the case of thermal transport takes the following form (e.g. [1]):

$$\mathbf{j}^M = - \frac{D^M c^M}{RT} \left(\nabla \mu^M + \frac{Q^M}{T} \nabla T \right) . \quad (5)$$

T is the absolute temperature and R is the gas constant. D^M , Q^M and μ^M are the diffusion coefficient, the heat of transport and the chemical potential of the diffusing substance, respectively. One may show that Q^M is related to the heat flux per unit mass flux of the diffusing substance in the absence of temperature gradient. Q^M depends on the solid and the diffusing substance, according to experimental measurements [1]. Relations (4) and (5) are valid in the deformed configuration. The respective relations in the reference configuration are given in [7].

Along parts of the boundary of the deforming solid, non-uniform temperature and/or heat flux is applied, causing heat flow within the solid. The governing equation of non-mechanical energy flow, in the deformed configuration, takes the form:

$$\rho c_p \frac{dT}{dt} = \left(\boldsymbol{\sigma} : \mathbf{D} - \frac{\rho}{\rho_0} \mathbf{S}^* : \frac{d\mathbf{E}^*}{dt} \right) +$$

$$- \frac{\rho}{\rho_0} T \frac{\partial \mathbf{E}^*}{\partial T} : \frac{d\mathbf{S}^*}{dt} - \mathbf{j}^M \cdot \nabla \mu^M + \nabla \cdot (k \nabla T) . \quad (6)$$

ρ and ρ_0 are the density of the solid in the deformed and reference configurations, respectively. c_p and k are the specific heat, at constant pressure, and the thermal conductivity of the solid, respectively. The term in parenthesis provides the heat generated by plastic deformation. The last term on the right corresponds to conducted heat, while the third term on the right corresponds to heat generated by diffusion. Finally the remaining term on the right is due to thermoelastic coupling. Therefore the variation of the heat content in the solid depends on conducted heat, on heat generated due to plastic deformation and mass diffusion and on thermoelastic coupling. Relation (6) clearly shows the coupling of non-mechanical energy flow, mass diffusion and elastic and plastic material deformation. If phase transformation occurs, a term, which corresponds to the change of entropy due to the phase transformation, must be added. Also phase transformation is generally associated with a stress-free expansion, which contributes to \mathbf{F}^* . This is the case of non-mechanical energy flow and hydrogen diffusion in hydride forming metals, when hydrides precipitate. Relation (6) can be used in hydrogen thermal transport problems of non-hydride forming metals, such as iron, nickel and aluminum. Relation (6) is also valid, without any modification, in hydride forming metals, such as niobium, vanadium, titanium, and zirconium, when hydride phase is not present.

The equivalent governing equation of non-mechanical energy flow in the reference configuration is the following:

$$\rho_0 c_p \frac{dT}{dt} = \left(\mathbf{S} : \frac{d\mathbf{E}}{dt} - \mathbf{S}^* : \frac{d\mathbf{E}^*}{dt} \right) +$$

$$- T \frac{\partial \mathbf{E}^*}{\partial T} : \frac{d\mathbf{S}^*}{dt} - \mathbf{J}^M \cdot \nabla_x \mu^M +$$

$$+ |\mathbf{F}| \left[\nabla_x (k \nabla_x T) \right] : (\mathbf{F}^{-1} \cdot \mathbf{F}^{-T}) . \quad (7)$$

$\nabla_x = \mathbf{b}_k \partial / \partial X_k$ is the gradient operator, defined on the reference configuration and calculated with respect to material coordinates. \mathbf{E} and \mathbf{S} are the total Lagrangian strain and the second Piola-Kirchhoff stress, respectively, both defined on the reference configuration, according to the well-known relations: $\mathbf{E} = (1/2)(\mathbf{F}^T \cdot \mathbf{F} - \mathbf{I})$, $\mathbf{S} = \mathbf{F}^{-1} \cdot \boldsymbol{\tau} \cdot \mathbf{F}^{-T}$.

\mathbf{J}^M is the flux of the diffusing substance, defined on the reference configuration; \mathbf{J}^M is related to the flux in the deformed configuration, as follows:

$$\mathbf{J}^M = |\mathbf{F}| \mathbf{F}^{-1} \cdot \mathbf{j}^M . \quad (8)$$

Relations (4-6) provide the governing equations, on the deformed configuration, of mass diffusion and non-mechanical energy flow in a metal under finite elastic-plastic deformation. Relations (6) and (7) are original. These relations are expected to contribute to the improvement of existing models (e.g. [5]), for the simulation of coupled mass-diffusion and non-mechanical energy flow, in areas where finite deformation is important. The derivation of relation (6) is discussed next.

DERIVATION OF NON-MECHANICAL ENERGY FLOW EQUATION

A caloric equation of state is assumed to exist, according to which, the local internal energy per unit mass of the solid, u , is determined by the thermodynamic state. The thermodynamic state is specified by the specific entropy, s , the thermodynamic substate variables, e_i , which are related to solid deformation, and the amount of the diffusing substance (moles) per unit solid mass, η^M (e.g. [19]):

$$u = u(s, e_i, \eta^M) . \quad (9)$$

$\eta^M = c^M / \rho$. The substate variables, e_i , are conjugate to thermodynamic tensions, τ_i . It is reminded that temperature, T , thermodynamic tensions, τ_i , and the chemical potential of the diffusing substance, μ^M , are defined as follows: $T = \partial u / \partial s$, $\tau_i = \partial u / \partial e_i$, $\mu^M = \partial u / \partial \eta^M$. Then:

$$\frac{du}{dt} = T \frac{ds}{dt} + \tau_i \frac{de_i}{dt} + \mu^M \frac{d\eta^M}{dt} . \quad (10)$$

According to the energy equation for the deforming solid (e.g. [19]):

$$\rho \frac{du}{dt} = \boldsymbol{\sigma} : \mathbf{D} - \nabla \cdot \mathbf{j}^E . \quad (11)$$

\mathbf{j}^E is the flux of non-mechanical energy, which includes both the flux of heat as well as the flux of energy, carried by the diffusing substance. \mathbf{j}^E is derived in the following, based on thermodynamics of irreversible processes [20].

Denbigh [20] presents a detailed discussion for the thermodynamic treatment of energy-flow/diffusion as well as of other coupled phenomena. His treatise for irreversible processes is based on Onsager's principle of microscopic reversibility. According to the empirical law of Fourier, heat flux is linearly related to the temperature gradient, which is the thermodynamic force, driving heat flow. In the case of diffusion in an isothermal system, the flux of a diffusing substance is proportional to the gradient of its chemical potential. Then, chemical potential gradient is the thermodynamic force driving diffusion under isothermal conditions. When the processes operate simultaneously, the coupling is taken into account by assuming that the non-mechanical energy and diffusing substance fluxes are linearly related to both thermodynamic forces:

$$\mathbf{j}^E = L^E \Delta^E + L^{EM} \Delta^M, \quad (12a)$$

$$\mathbf{j}^M = L^{ME} \Delta^E + L^M \Delta^M, \quad (12b)$$

$$L^{EM} = L^{ME}. \quad (12c)$$

Δ^E and Δ^M are the thermodynamic forces driving non-mechanical energy flow and mass diffusion, respectively. L^E , L^M , L^{EM} and L^{ME} are phenomenological coefficients. Relation (12c) is valid due to Onsager's reciprocity relation. The thermodynamic forces, when multiplied by the respective fluxes, produce the rate of internal generation of entropy per unit volume, ψ , which is caused by mass diffusion and non-mechanical energy flow [20]:

$$T\psi = \mathbf{j}^E \cdot \Delta^E + \mathbf{j}^M \cdot \Delta^M. \quad (13)$$

In order to derive \mathbf{j}^E , the thermodynamic forces and the phenomenological coefficients need to be calculated. The thermodynamic forces, Δ^E and Δ^M , are calculated first.

Substitutions of the energy equation, (11), and the equation of mass conservation of the diffusing substance, (4), into (10) lead to the following relation:

$$\begin{aligned} \rho \frac{ds}{dt} + \nabla \cdot \left(\frac{\mathbf{j}^E - \mu^M \mathbf{j}^M}{T} \right) &= \frac{1}{T} \left(\boldsymbol{\sigma} : \mathbf{D} - \rho \tau_i \frac{de_i}{dt} \right) + \\ &+ \frac{1}{T} \left[-\frac{\mathbf{j}^E}{T} \cdot \nabla T - T \mathbf{j}^M \cdot \nabla \left(\frac{\mu^M}{T} \right) \right]. \end{aligned} \quad (14)$$

Let one define:

$$\psi_1 = \frac{1}{T} \left(\boldsymbol{\sigma} : \mathbf{D} - \rho \tau_i \frac{de_i}{dt} \right), \quad (15a)$$

$$\psi_2 = \frac{1}{T} \left[-\frac{\mathbf{j}^E}{T} \cdot \nabla T - T \mathbf{j}^M \cdot \nabla \left(\frac{\mu^M}{T} \right) \right], \quad (15b)$$

$$\mathbf{s} = \frac{\mathbf{j}^E - \mu^M \mathbf{j}^M}{T}, \quad (15c)$$

Then by integrating (14) over the volume of the solid, which in the deformed configuration is V bounded by the surface S , one derives:

$$\frac{d}{dt} \int_V \rho s dV + \int_S \mathbf{s} \cdot \mathbf{n} dS = \int_V (\psi_1 + \psi_2) dV. \quad (16)$$

The first term in (16) is the rate of entropy of the specified volume. The second term in (16) is the rate of entropy, flowing out of the volume V , due to heat flux on the boundary. The right-hand side term in (16) is the rate of the internal generation of entropy. Consequently the integrand of the right-hand side term is equal to the rate of internal generation of entropy per unit volume, ψ , also given by (13). Therefore combination of (15a), (15b) and (13) yields the thermodynamic forces Δ^E and Δ^M :

$$\Delta^E = -\frac{1}{T} \nabla T, \quad (17a)$$

$$\Delta^M = -T \nabla \left(\frac{\mu^M}{T} \right). \quad (17b)$$

Relations (17a) and (17b) are identical to relations (2.2a) and (2.2b), which were derived by the author in the case of hydrogen diffusion and heat conduction in metals, under infinitesimal displacement gradient deformation [5] (see also relations (2.13a) and (2.13b) in [4]).

The derivation of \mathbf{j}^E is completed, when the phenomenological coefficients L^E and L^{EM} are calculated. For this purpose one considers relation (5) for the flux of a diffusing mass in the case of thermal transport. When (5) is compared with (12b), the coefficients L^M and L^{EM} are derived:

$$L^M = \frac{D^M c^M}{RT}, \quad (18a)$$

$$L^{EM} = \frac{D^M c^M (\mu^M + Q^M)}{RT}. \quad (18b)$$

The last unknown coefficient, L^E , is calculated by considering the case of heat conduction, under no mass diffusion:

$$\mathbf{j}^E = -k \nabla T. \quad (19)$$

In this case, in which the flux of the diffusing substance is zero, the following relation is also valid, according to (5):

$$\nabla \mu^M = -\frac{Q^M}{T} \nabla T. \quad (20)$$

Manipulation of (12a), by using (17a), (17b), (18b), (19) and (20), leads to the expression of L^E :

$$L^E = kT + \frac{D^M c^M (\mu^M + Q^M)^2}{RT}. \quad (21)$$

By substituting (21) and (18b) into (12a) one derives the general relation of non-mechanical energy flux, when heat conduction and mass diffusion operate simultaneously:

$$\mathbf{j}^E = (\mu^M + Q^M) \mathbf{j}^M - k \nabla T. \quad (22)$$

The term $Q^M \mathbf{j}^M$ is the heat flux caused by diffusion, while $-k \nabla T$ is the heat flux, due to heat conduction in the solid. The term $\mu^M \mathbf{j}^M$ is the flux of the energy of the diffusing substance. Thus the use of the term of non-mechanical energy flux, instead of heat flux, for \mathbf{j}^E , is explained. It is emphasized that relation (22), which is valid in the deformed configuration, is identical to the respective relation for hydrogen diffusion and heat conduction in a metal, under infinitesimal displacement gradient deformation, when the quantities are interpreted appropriately (see [4], [5]). Note

that, according to (22), in the absence of temperature gradient, the heat flux per unit mass flux of the diffusing substance, $|\mathbf{j}^E - \mu^M \mathbf{j}^M|/|\mathbf{j}^M|$, is equal to the absolute value of the heat of transport, $|Q^M|$.

One may choose the components of the Lagrangian strain \mathbf{E}^* as the substate variables e_i , in which case the conjugate thermodynamic tensions, τ_i , are given by the components of \mathbf{S}^*/ρ_0 . Then, by taking also into account (22), (14) leads to the following relation:

$$\rho T \frac{ds}{dt} = \left(\boldsymbol{\sigma} : \mathbf{D} - \frac{\rho}{\rho_0} \mathbf{S}^* : \frac{d\mathbf{E}^*}{dt} \right) + \nabla \cdot (k \nabla T) - Q^M \nabla \cdot \mathbf{j}^M - \mathbf{j}^M \cdot \nabla \mu^M. \quad (23)$$

It is reminded that temperature, T , and thermodynamic tensions, τ_i , are functions of the thermodynamic state, i.e. $T = T(s, e_i, \eta^M)$ and $\tau_j = \tau_j(s, e_i, \eta^M)$. The assumption of invertibility of the functions of temperature and thermodynamic tensions leads to $s = s(T, \tau_i, \eta^M) = s(T, \mathbf{S}^*, \eta^M)$ and therefore:

$$\begin{aligned} \frac{ds}{dt} &= \frac{\partial s}{\partial T} \frac{dT}{dt} + \frac{\partial s}{\partial \mathbf{S}^*} : \frac{d\mathbf{S}^*}{dt} + \frac{\partial s}{\partial \eta^M} \frac{d\eta^M}{dt} = \\ &= \frac{c_{S^*}}{T} \frac{dT}{dt} + \frac{1}{\rho_0} \frac{\partial \mathbf{E}^*}{\partial T} : \frac{d\mathbf{S}^*}{dt} - \frac{Q^M}{\rho T} \nabla \cdot \mathbf{j}^M. \end{aligned} \quad (24)$$

c_{S^*} is the specific heat of the solid at constant thermodynamic tensions. c_{S^*} is assumed equal to the specific heat of the solid at constant pressure, c_p . In deriving (24) it was taken into account that the variation of entropy with respect to the concentration of the diffusing substance is equal to the ratio of the heat of transport of the diffusing substance over temperature:

$$\frac{\partial s}{\partial \eta^M} = \frac{Q^M}{T}, \quad (25)$$

as well as that $d\eta^M/dt = -(1/\rho) \nabla \cdot \mathbf{j}^M$. Finally, by substituting (24) into (23), one derives the governing equation of non-mechanical energy flow (6).

CONCLUSIONS

The governing equation of the flow of non-mechanical energy, which includes conducted heat and energy transported by mass diffusion, is derived in the case of a metallic

solid under finite deformation. The coupling of non-mechanical energy flow, mass diffusion and elastic-plastic solid deformation is rigorously taken into account. According to the analysis, the variation of the heat content of the solid depends on conducted heat, on heat generated due to plastic deformation and mass diffusion and on thermoelastic coupling. Both forms of the governing equation on the reference (non-deformed) and the deformed configurations are given. Besides its general validity, the present derivation provides the information for further progressing existing mathematical models [3-5], which are based on infinitesimal displacement gradient theory. It is therefore expected to contribute to the precise simulation of hydrogen-induced embrittlement and fracture in metals, under conditions of thermal transport, in the area ahead of the tip of a stationary crack or a crack, which starts growing, i.e. in the area where the consideration of finite deformation is necessary.

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