

# ELASTICITY, PLASTICITY, RHEOLOGY AND THERMAL STRESS — AN IRREVERSIBLE THERMODYNAMICAL THEORY

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## ABSTRACT

We present a thermodynamical formulation of elastic, plastic, rheological and thermal stress phenomena of solids that is based on two pillars. One of them is a recent novel definition of kinematic quantities that enables the description of finite deformation elastic, plastic and thermal expansion changes in an automatically objective way. In parallel, the other pillar is irreversible thermodynamics. We show how naturally the well-known aspects of plasticity, as well as the inclusion of rheology, meet the requirement of positive definite entropy production. The general framework is illustrated via a simulation example and an experimental example.

## INTRODUCTION

In nonquantitative/heuristic terms, objectivity may be formulated as the requirement that the physical content of a theory must be independent from the description used for the formulation of the theory. It might be expected that it is nontrivial to ensure objectivity for a theory, and paradoxes, controversies and errors indicate that indeed this is the case.

Motivated by the need for a safely objective formulation of continuum physics, in a recent work, we have introduced a novel definition of kinematic quantities [1; 2]. By working on Galilean spacetime directly, it was possible to avoid the use of any auxiliary element—reference frame, reference time, reference configuration etc.—, which are sources of possible violation of objectivity in the conventional approaches. In our framework, all kinematic quantities and equations are automatically objective.

The logical continuation of this program is to reformulate the mechanical and thermodynamical theories in terms of these quantities, as well as to look for possible improvements and possibly emerging new opportunities for theory building. The present work reports on results obtained in this direction. We show here a small deformation thermodynamical framework for elastic, plastic, thermal expansion and rheological phenomena of solids. Our original aim was an illustration of that, with the spacetime-based quantities, one can express anything that is needed in continuum physics. In parallel, it has gradually turned out that these quantities enable and suggest some such improvements and possibilities in continuum physics that have not been apparent before.

To see how our thermodynamical theory performs in practice, we provide here two illustrations, a numerical calculation of a concrete example process and an experiment, where the results demonstrate the features of the theoretical framework.

## KINEMATIC QUANTITIES

Based on Matolcsi's reference frame free approach to theoretical physics [3; 4; 5], the problems of objectivity and material frame indifference [6; 7; 8; 9; 10] have been investigated in a series of papers [11; 12; 13; 14; 1]. In particular, in [1], the kinematic quantities for elastic and plastic processes of solids have been presented in a way that is free from any auxiliary elements like reference frame, reference time and reference configuration. During the birth of [1], it has been realized that this new approach incorporates thermal expansion also in a natural way and reveals some nontrivial kinematic and dynamical consequences of thermal expansion [2].

This kinematic background of the subsequent thermodynamical framework can be summarized as follows.

### The motion of the continuum

The continuum is considered as a three dimensional smooth manifold. Each material point of it moves along a smooth world line in spacetime—which we will take here as a Galilean (“non-relativistic”) spacetime—, at time  $t$ , the spacetime location of  $P$  is  $r_t(P)$ . Its material gradient  $\tilde{\nabla}$ , *i.e.*, the derivative with respect to the variable  $P$ ,

$$\mathbf{J}_t(P) := (r_t \otimes \tilde{\nabla})(P), \quad (1)$$

is the world line gradient (and is the spacetime compatible generalization of the traditional deformation gradient) [spatial derivatives will act to the left or to the right according to the context, always to indicate the correct tensorial order]. This tensor maps tangent vectors of the material manifold to spacelike spacetime vectors, which form a three dimensional Euclidean vector space with Euclidean scalar product  $\mathbf{h}$ . At any instant  $t$ , the current spatial distance of two material points  $P, Q$  is the

distance of  $r_t(P)$  and  $r_t(Q)$  with respect to the spatial Euclidean metric  $\mathbf{h}$ ,

$$d_t(P, Q) = \|r_t(Q) - r_t(P)\|_{\mathbf{h}}. \quad (2)$$

This induces a current metric

$$\tilde{\mathbf{h}}_t := \mathbf{J}_t^T \mathbf{h} \mathbf{J}_t \quad (3)$$

on the material manifold ( $^T$  standing for transpose), a scalar product for the tangent vectors at each material point.

The spacetime velocity of material point  $P$  at  $t$  is the time derivative  $\dot{r}_t(P) = v_t(P)$ . If we change from the Lagrangian/material/comoving variable to the Eulerian/spacetime variable then the material gradient  $\tilde{\nabla}$  is mapped to the spatial spacetime derivative  $\nabla$  via  $\mathbf{J}_t$ , and we find

$$\mathbf{L}_t = \dot{\mathbf{J}}_t \mathbf{J}_t^{-1} \quad (4)$$

for the velocity gradient

$$\mathbf{L}_t(P) := (v_t \otimes \tilde{\nabla})(P). \quad (5)$$

(Naturally, the substantial/comoving time derivative coincides with the partial time derivative in the Lagrangian picture.)

### Elasticity

So far, our continuum could have been a solid as well as a liquid (and even a laminarly flowing gas). What could be the mathematical formulation of the distinction between a solid and a liquid? Expressing that ‘a solid has a structure’, we can say that a solid possesses a self-metric (natural metric) structure, with which its current metric coincides when the solid is under no external influence. Namely, we assign to a solid a certain metric  $\tilde{\mathbf{g}}$  on the material manifold. This metric tells the distances of material points—*i.e.*, coincides with the current metric  $\tilde{\mathbf{h}}_t$ —when the solid is relaxed.

Our intention with an elastic kinematic quantity is to be the variable on which elastic stress depends, which, under classical mechanical experience, may be expected to depend on the distances between nearby material points. Taking into account that  $\tilde{\mathbf{g}}$  describes the distances in unstressed state, the elastic kinematic quantity could measure the deviation of the current metric  $\tilde{\mathbf{h}}_t$  from the self-metric  $\tilde{\mathbf{g}}$ . To this end, we can define

$$\tilde{\mathbf{A}}_t := \tilde{\mathbf{g}}^{-1} \tilde{\mathbf{h}}_t \quad (6)$$

(elastic shape tensor), which proves to be the spacetime compatible generalization of the ‘right’ Cauchy-Green tensor, and

$$\tilde{\mathbf{D}}_t := \ln \sqrt{\tilde{\mathbf{A}}_t} = \frac{1}{2} \ln \tilde{\mathbf{A}}_t \quad (7)$$

(elastic deformedness tensor), which is the generalization of the ‘right’ Hencky strain.

These tensors have been defined on the material manifold—acting on material tangent vectors—but can be transported to spacetime via  $\mathbf{J}$ . For the spacetime version (the ‘left’ version), we can derive the evolution equation

$$\dot{\mathbf{A}} = \mathbf{L}\mathbf{A} + \mathbf{A}\mathbf{L}^T. \quad (8)$$

### Thermal expansion

As far as elasticity is concerned, the relaxed metric can be regarded as a constant tensor. However, we are aware of physical phenomena where the structure of a solid changes, where its relaxed distances change. One such phenomenon is thermal expansion. Restricting ourselves to isotropic solids, if  $l(T)$  denotes a characteristic length (edge length of a cube, or radius of a sphere) of a unit amount (mass, or molar number) of the material at temperature  $T$  then, for the temperature dependence of the relaxed metric, we have

$$\tilde{\mathbf{g}}(T_2) = \left( \frac{l(T_2)}{l(T_1)} \right)^2 \tilde{\mathbf{g}}(T_1) \quad (9)$$

[in accord with that the metric expresses squared distances]. The usual definition of the linear thermal expansion coefficient is

$$\alpha(T) := \frac{dl(T)/dT}{l(T)}. \quad (10)$$

When temperature changes in time at a material point, we have

$$\dot{\tilde{\mathbf{g}}} = \left( \frac{d}{dT} \tilde{\mathbf{g}} \right) \dot{T} = 2\alpha(T) \dot{T} \tilde{\mathbf{g}} \quad (11)$$

following from Eq. (9), implying

$$\dot{\mathbf{A}} = \mathbf{L}\mathbf{A} + \mathbf{A}\mathbf{L}^T - 2\alpha\mathbf{A}. \quad (12)$$

Let us note that, in a theory,  $l(T)$ , and thus  $\alpha(T)$ , must be given constitutively.

### Plasticity

Another phenomenon where the structure of a solid changes is plasticity. Therefore, plasticity is another source of  $\dot{\tilde{\mathbf{g}}} \neq \mathbf{0}$ . Putting elasticity, thermal expansion and plasticity together, we have

$$\dot{\mathbf{A}} = \mathbf{L}\mathbf{A} + \mathbf{A}\mathbf{L}^T - 2\alpha\mathbf{A} - 2\mathbf{Z}, \quad (13)$$

where  $\mathbf{Z}$ , the plastic change rate tensor is responsible for the additional change rate of  $\tilde{\mathbf{g}}$ , and is also to be given constitutively.

### Remarks

We can see that, actually,  $\tilde{\mathbf{g}}$  is not purely a kinematic quantity. Still, since elastic, plastic and thermal expansion deformations are traditionally considered as kinematic, we must speak about it here, where these kinematic definitions are given. Also,  $\tilde{\mathbf{g}}$  is not purely dynamical, either.

As another remark, useful for the applications, strain can be defined only with respect to a reference time  $t_0$ , as

$$\mathbf{E}_{t_0 \rightarrow t} := \int_{t_0}^t \mathbf{L}^S \tilde{\mathbf{g}} dt, \quad (14)$$

where  $\overset{\text{S}}{\mathbf{D}}$  denotes symmetric part and  $\widetilde{d}t$  indicates comoving integration. In parallel, the conventional deformation gradient can be expressed in the present formalism as

$$\mathbf{F}_{t_0 \rightarrow t} = \mathbf{J}_t \mathbf{J}_{t_0}^{-1}, \quad (15)$$

and satisfies

$$\mathbf{A}_t = \mathbf{F}_{t_0 \rightarrow t} \mathbf{A}_{t_0} \mathbf{F}_{t_0 \rightarrow t}^T. \quad (16)$$

### Small deformation

From now on, we restrict our treatment to the small deformation regime, where (i)  $\mathbf{A}$  is near to  $\mathbf{I}$ , thus also satisfying  $\mathbf{A} \approx \mathbf{I} + 2\mathbf{D}$ , (ii)  $\mathbf{J}$  does not change considerably during the time scale on which we consider a process, and (iii)  $\alpha$  can also be regarded as a constant. Then Eq. (13) simplifies, in leading order, to

$$\dot{\mathbf{A}} = \mathbf{L} + \mathbf{L}^T - 2\alpha\mathbf{I} - 2\mathbf{Z}, \quad (17)$$

rearrangeable as

$$\mathbf{L}^S = \dot{\mathbf{D}} + \alpha\dot{T}\mathbf{1} + \mathbf{Z}. \quad (18)$$

A consequence of the small deformation approximation is that we do not have to pay attention to the difference between ‘right’ and ‘left’, *i.e.*, material and spacetime tensorial quantities.

## MECHANICS AND THERMODYNAMICS

### Stress

Let us start building the dynamical theory by choosing what we expect on the mechanical side: let our elastic constitutive equation be the simple linear one:

$$\boldsymbol{\sigma} = U^d \mathbf{D}^d + U^s \mathbf{D}^s \quad (19)$$

with

$$\mathbf{D}^s = \frac{1}{3}(\text{tr}\mathbf{D})\mathbf{1}, \quad \mathbf{D}^d = \mathbf{D} - \mathbf{D}^s, \quad U^s = 3K, \quad U^d = 2G. \quad (20)$$

Actually, a nonlinear choice could also be incorporated, but let us now pursue a simple, yet interesting, setting.

At this point, we can already observe that the classic Duhamel-Neumann formula for thermoelasticity [15] is recovered as a special case. To see this, we must assume what are assumed there: that, at an initial time  $t_0$ , the temperature is  $T_0$  and elastic deformedness is considered zero ( $\mathbf{D}_{t_0} = \mathbf{0}$ ,  $\mathbf{A}_{t_0} = \mathbf{I}$ ), that is, we start with an unstressed, relaxed, natural initial state. We also stay in the small deformation regime, and neglect plastic changes. Then, at time  $t$ , in the leading order approximation,

$$\begin{aligned} \mathbf{D}_t &= \frac{1}{2}(\mathbf{A}_t - \mathbf{I}) = \frac{1}{2}(\mathbf{F}_{t_0 \rightarrow t} \mathbf{F}_{t_0 \rightarrow t}^T - \mathbf{I}) \\ &= \mathbf{E}_{t_0 \rightarrow t} - \alpha(T - T_0)\mathbf{I}. \end{aligned} \quad (21)$$

Inserting this into Eq. (19) yields

$$\boldsymbol{\sigma}_t \approx 2G\mathbf{E}_{t_0 \rightarrow t} + (K - \frac{2}{3}G)(\text{tr}\mathbf{E}_{t_0 \rightarrow t})\mathbf{I} - 3K\alpha(T - T_0)\mathbf{I}, \quad (22)$$

which is precisely the Duhamel-Neumann expression.

### Thermodynamical quantities for elasticity, thermal expansion and plasticity

Our first step towards thermodynamics is that we expect the first law to be satisfied:

$$\rho\dot{u} = -\mathbf{j}_u \cdot \nabla + \boldsymbol{\sigma} : \mathbf{L}^S \quad (23)$$

for the specific internal energy  $u$  and its current  $\mathbf{j}_u$ , both to be specified constitutively later (and the density  $\rho$  being constant in the small deformation regime) [ $\text{tr}$  denotes trace]. Let us then construct the rest of the thermodynamical build-up as follows: our aim is to rewrite Eq. (23) assuming  $\mathbf{j}_s = \mathbf{j}_u/T$  for the entropy current  $\mathbf{j}_s$ , and with an appropriate specific entropy  $s(\mathbf{D}, T)$ , as

$$T\rho\dot{s} = T(-\mathbf{j}_s \cdot \nabla + \boldsymbol{\sigma}_s), \quad (24)$$

where the positive definiteness of the entropy production,  $\boldsymbol{\sigma}_s \geq 0$  is also to be ensured constitutively.

If we choose again a simple internal energy function, *i.e.*, consisting of an elastic energy part and a thermal term corresponding to a constant specific heat  $c$ ,

$$u = cT + \frac{U^d}{2\rho} \mathbf{D}^d : \mathbf{D}^d + \frac{U^s}{2\rho} \mathbf{D}^s : \mathbf{D}^s + \frac{U^s}{\rho} T \alpha \text{tr} \mathbf{D}^s, \quad (25)$$

then, omitting the straightforward details, that appropriate entropy function proves to be

$$s = c \ln \frac{T}{T_0} + \frac{U^s}{\rho} \alpha \text{tr} \mathbf{D}^s + s_0 \quad (26)$$

with any temperature value  $T_0$  and constant  $s_0$ , and the corresponding entropy production is found to be

$$\boldsymbol{\sigma}_s = \nabla \frac{1}{T} \cdot \mathbf{j}_u + \frac{1}{T} \boldsymbol{\sigma} : \mathbf{Z} = \nabla \frac{1}{T} \cdot \mathbf{j}_u + \frac{U^d}{T} \mathbf{D}^d : \mathbf{Z} + \frac{U^s}{T} \mathbf{D}^s : \mathbf{Z}. \quad (27)$$

Our remaining task is to ensure the positive definiteness of the latter.

One simple choice guaranteeing this is when we take the standard constitutive formula for heat conduction,

$$\mathbf{j}_u = \lambda \nabla \frac{1}{T} \quad (28)$$

(with, say, a constant positive  $\lambda$ ), and prescribe the plastic constitutive equation as

$$\mathbf{Z} = \Gamma \dot{\mathbf{D}}^d \quad \text{with} \quad \Gamma = \gamma H \left( \mathbf{D}^d : \mathbf{D}^d - B \right) H \left( \mathbf{D}^d : \dot{\mathbf{D}}^d \right), \quad (29)$$

where  $\gamma$  and  $B$  are positive constants, and  $H$  is the Heaviside function.

The choice Eq. (29) is fairly plausible from the plasticity point of view: the plastic change rate is deviatoric and is proportional to the elastic change rate, the first Heaviside term describes a von Mises yield criterion (recall that stress is in a linear relationship with  $\mathbf{D}$ ), and the second Heaviside term expresses the natural expectation that plastic change is switched off during unloading.

On the other, thermodynamical, side, the second Heaviside term ensures that entropy production is positive definite. One may actually dare to put this reversely: plasticity must be switched off during unloading, as otherwise positive definiteness of entropy production would be violated.

We remark that it poses no difficulty to incorporate temperature dependent coefficients  $U^s$ ,  $U^d$ ,  $\alpha$ ,  $c$ .

### Adding rheology

The thermodynamical formulation of rheological models is possible with the aid of internal variables (dynamical degrees of freedom [16]). The details [17] of this derivation cannot be given here, but the outline is similar to what happens in [18].

Namely, we assume the presence of an additional internal variable, a symmetric tensor  $\xi$ , and extend our previous entropy function as

$$s = s_{\text{previous}} - \frac{1}{2} \xi : \xi. \quad (30)$$

If plasticity and thermal expansion are neglected then the positive definiteness of entropy production leads to, in the linear Onsagerian setting, after eliminating the internal variable, a linear rheological model with  $\sigma$ ,  $\dot{\sigma}$ ,  $\mathbf{D}$ ,  $\dot{\mathbf{D}}$ ,  $\ddot{\mathbf{D}}$  terms. Therefore, we arrive at a common generalization of the Poynting–Thomson–Zener and the Jeffreys models, which we may call the inertial Poynting–Thomson–Zener model.

### A SIMULATION

The evolution equations Eq. (18), Eq. (23), together with the approximate mechanical equation of motion

$$\sigma \cdot \nabla = 0 \quad (31)$$

and the constitutive prescriptions Eq. (19), Eq. (25), Eq. (28), Eq. (29), form a closed set of equations, thus being capable to calculate a concrete process. To demonstrate this, we have performed a numerical calculation for a cylindrical rod uniaxially stretched by an increasing force, linear in time.

Figure 1. shows the strains and the temperature as the function of time. Plastic change (blue line) begins only above the critical stress. Below this, temperature decreases, similarly to what happens for an adiabatically expanded gas. Therefore, the total strain (black line) runs a bit below the elastic strain (green line), the difference caused by the nonzero thermal expansion coefficient. When the plastic change also appears, the total strain increases faster, and, due to the dissipative power term  $\sigma : \mathbf{Z}$ , temperature also starts to increase.

Figure 2. shows the modification of the setup, where the rod has slightly nonconstant cross section: then plasticity (blue

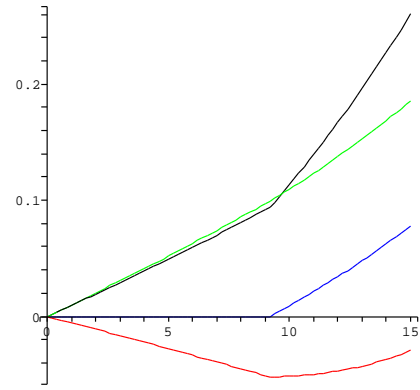


Figure 1. Uniaxially stretched rod. The temperature (red line) first decreases and then increases, the elastic strain (green line) increases following the increased stress, the plastic strain (blue line) appears only above the critical stress, causing that the total strain (black line) starts to increase faster.

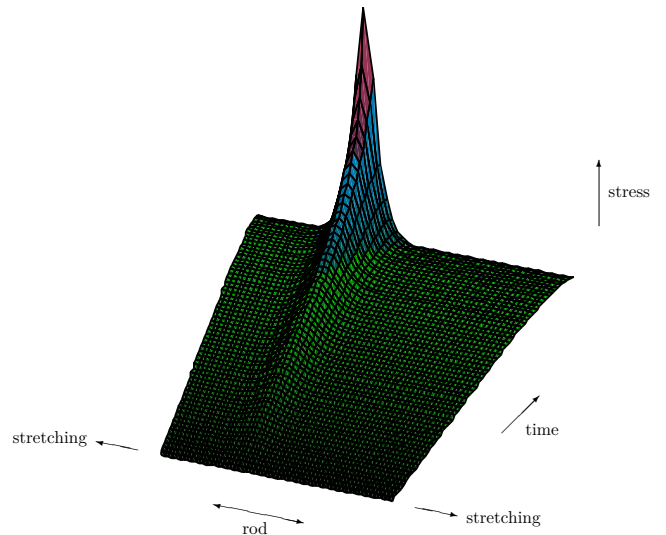


Figure 2. Stretching a rod with slightly nonconstant cross section. Plastic change (blue region) starts where the rod is the thinnest, and failure (red region) also occurs there, the remaining part of the rod has only elastic and thermal expansion deformations (green region).

region) appears first at the location where the sample is thinner, and failure (red region) would also appear there, if a simple stress failure criterion is added for illustration and for the sake of the following Section.

### AN EXPERIMENT

We have carried out the above stretching example not only in simulation but also as an experiment on a plastic (“Docamid 6G-H” polyamide) sample. In addition to measuring the extensions, a thermal camera has measured the surface temperature of the sample during the process. We can observe on the snapshots in Fig. 3 the initial decrease of temperature and then its increase, observable where plastic change has already started.

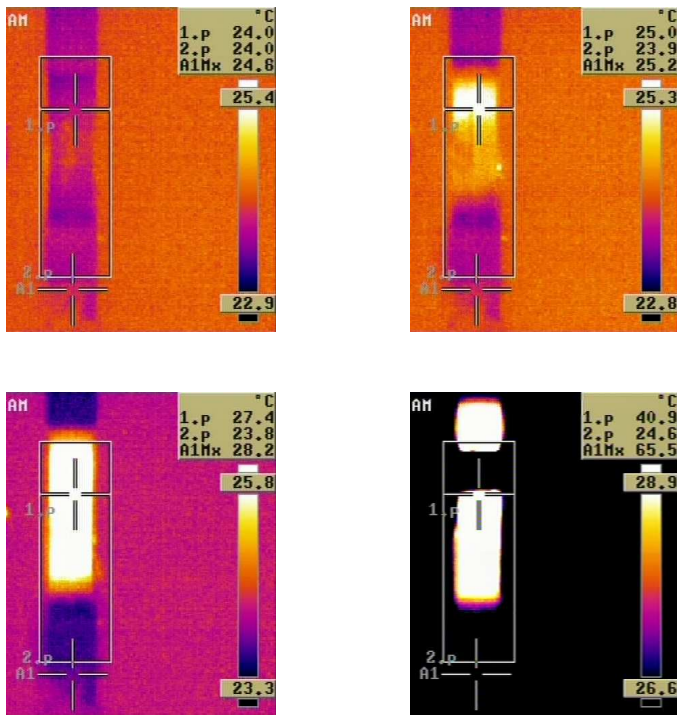
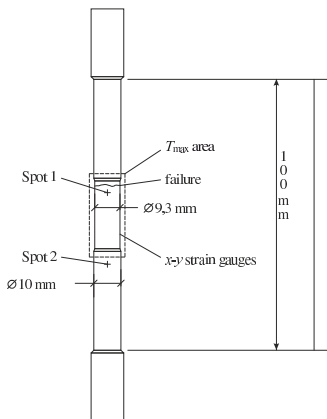


Figure 3. Stretching a rod with slightly nonconstant cross section — experiment. The outline (upper left figure) displays the two spots whose temperature was not only recorded by the thermal camera but also numerically displayed, together with the maximal temperature in the rectangle area. The subsequent five figures are snapshots taken by thermal camera. The first shows the initial state, then the quasi-adiabatic cooling is observable, then heat dissipation appears due to plastic change, then the plastic change reaches the whole thinner part of the sample, and finally failure occurs.

## CONCLUSION

We intended to illustrate that our recent kinematic formulation can be incorporated in mechanical and thermodynamical theories, with thermal expansion and plastic processes described naturally and realistically, even when considering only simple constitutive choices and small deformations. Rheology can also be added—when plasticity and thermal expansion are also kept then interesting cross effects are expected to emerge, offering new theoretical possibilities for explaining experimental observations.

The finite deformation version of the presented theory is also possible, though some formulae become nontrivial due to the

fact that the multiplication of tensors is not commutative. This work is in progress currently. Finally, we wish to strengthen the connection between theory and experiment, evaluating quantitatively the already performed experiments and to devise new ones.

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## REFERENCES

- [1] T. Fülöp and P. Ván, Kinematic Quantities of Finite Elastic and Plastic Deformation, *Math. Meth. Appl. Sci.*, vol. 35, pp. 1825–1841, 2012.
- [2] T. Fülöp, Thermal Expansion, Elastic Stress and Finite Deformation Kinematics, in: Proceedings of the 10th HEEP International Conference, 23–25 May 2011, Balatonfüred, Hungary. Published by: Budapest University of Technology and Economics, Department of Energy Engineering, 2011, pp. 227–232.
- [3] T. Matolcsi, *A Concept of Mathematical Physics: Models for SpaceTime*, Akadémiai Kiadó (Publishing House of the Hungarian Academy of Sciences), Budapest, 1984.
- [4] T. Matolcsi, *A Concept of Mathematical Physics: Models in Mechanics*, Akadémiai Kiadó (Publishing House of the Hungarian Academy of Sciences), Budapest, 1986.
- [5] T. Matolcsi, *Spacetime Without Reference Frames*, Akadémiai Kiadó Publishing House of the Hungarian Academy of Sciences), Budapest, 1993.
- [6] G. Ryskin, Misconception Which Led to the "Material Frame Indifference" controversy, *Physical Review E*, vol. 32(2), pp. 1239–1240, 1985.
- [7] M. E. Gurtin, E. Fried, and L. Anand, *The Mechanics and Thermodynamics of Continua*, Cambridge University Press, 2010.
- [8] A. I. Murdoch, Objectivity in classical continuum physics: a rationale for discarding the 'principle of invariance under superposed rigid body motions' in favour of purely objective considerations, *Continuum Mechanics and Thermodynamics*, vol. 15, pp. 309–320, 2003.
- [9] W. Noll, A Frame Free Formulation of Elasticity, *Journal of Elasticity*, vol. 83, pp. 291–307, 2006.
- [10] M. Frewer, More Clarity on the Concept of Material Frame-indifference on Classical Continuum Mechanics, *Acta Mechanica*, vol. 202, pp. 213–246, 2009.
- [11] T. Matolcsi, On Material Frame-indifference, *Archive for Rational Mechanics and Analysis*, vol. 91(2), pp. 99–118, 1986.
- [12] T. Matolcsi and T. Gruber, Spacetime Without Reference Frames: An Application to the Kinetic Theory, *International Journal of Theoretical Physics*, vol. 35(7), pp. 1523–1539, 1996.
- [13] T. Matolcsi and P. Ván, Can Material Time Derivative Be Objective? *Physics Letters A*, vol. 353, pp. 109–112, 2006.
- [14] T. Matolcsi and P. Ván, Absolute Time Derivatives, *Journal of Mathematical Physics*, vol. 48, No. 053507–19, 2007.
- [15] V. A. Lubarda, On Thermodynamic Potentials in Linear Thermoelasticity, *International Journal of Solids and Structures*, vol. 41(7), pp. 7377–7398, 2004.
- [16] J. Verhás, *Thermodynamics and Rheology*, Akadémiai Kiadó and Kluwer Academic Publisher, Budapest, 1997.

[17] P. Ván and T. Fülöp, Classic and New Rheological Models in the Framework of a Thermodynamical Internal Variable Theory, in preparation.

[18] P. Ván and T. Fülöp, Universality in Heat Conduction Theory: Weakly Nonlocal Thermodynamics, *Annalen der Physik*, vol. 524, 470–478, 2012.