# MÜLLER'S K VECTOR IN THERMOELASTICITY.

JÓZSEF VERHÁS

Abstract. The concept of the $\vec{K}$ vector first proposed by I. Müller [1] made revolutionary changes in irreversible thermodynamics. It may be important also in the theory of thermoelasticity. The well known theories are based on thermal expansion, and the recent improvements are looked for in the theory of heat conduction. The reason is that heat conduction is accounted with scalar and vector variables while elasticity with second order tensors and there is no direct linear coupling between second order tensors and vectors or scalars in an isotropic material. The deviations from the present theories urge new pathways for research. Such a new track can be opened by Onsager's thermodynamics supplemented with dynamic degrees of freedom. This theory is usually referred to as extended thermodynamics. The key moment is in the general form of the entropy current out of local equilibrium, which leads to the formal introduction of the transport of the dynamic degrees of freedom. The skeleton of the possible theories is based on the introduction of one or more vectorial dynamic variables. They can be coupled to the current density of the heat flow, while their 'diffusion' intensities are second order tensors coupled directly in linear order to the stress tensor even if the material is isotropic. The possibilities are demonstrated on an example with one dynamic degree of freedom. The new theory may explain why a thin coat of mortar can prevent the disintegration of the rock in a tunnel.

## Introduction

Non-equilibrium thermodynamics has been applied with success to a lot of phenomena even in the form that nowadays is referred to as "classical irreversible thermodynamics"—in the form that was accepted just after the first papers of Onsager [2–5] and is presented—more or less strictly—in the classical monographs [6–9]. It concerned the principle of local equilibrium. The latter turned out to be too tight and was generalized [10–15]. The departure from local equilibrium turned out very fruitful and opened a broad perspective of applications [16–26]. Here a model for thermal stress is sketched that may be the closest to the original Onsagerian presentation. In the model, thermal stress is invoked by heat conduction through linear Onsager equations.

---

*Key words and phrases.* thermodynamic modeling, Onsager–Casimir reciprocal relation, irreversible thermodynamics, thermoelasticity.

Supported by OTKA 62278 and T04848.

## 1. The model

Assume a moving solid body in which heat conduction is present. The first law reads

$$\rho\dot{u} + \operatorname{div}\vec{J}_q = \boldsymbol{t} : \mathring{\boldsymbol{d}}. \tag{1.1}$$

Here $\rho$ is the density, $u$ the specific internal energy, $\vec{J}_q$ the current density of heat flow, $\boldsymbol{t}$ Cauchy's stress, and $\mathring{\boldsymbol{d}}$ the symmetric part of the velocity gradient. The $^\circ$ above the symbols means co-rotational derivative. Further on the study will be restricted to small deformations for the sake of simpler formulae; with this restriction, the co-rotational derivative of the dilatation tensor $\boldsymbol{d}$ equals the symmetric part of the velocity gradient.

The local state variables are the specific internal energy $u$, the dilatation tensor $\boldsymbol{d}$, and a vectorial dynamic variable $\vec{\xi}$ not yet specified. As the variable $\vec{\xi}$ is determined by the others at an equilibrium state they can be chosen in a special way so that the entropy function takes the form

$$s = s^e\left(u - \frac{1}{2}\vec{\xi}^{\,2}, \boldsymbol{d}\right). \tag{1.2}$$

Here $s^e(u, \boldsymbol{d})$ is the equilibrium entropy function. The choice of the dynamic variables resulting the above non-equilibrium entropy function is ensured by the Morse–lemma [27] and the maximum property of the entropy.

The general form of the entropy balance reads

$$\rho\dot{s} + \operatorname{div}\vec{J}_s = \sigma_s \geq 0 \tag{1.3}$$

Here $\vec{J}_s$ is the entropy flow density and $\sigma_s$ the entropy production. The inequality expresses the second law.

The system is not in local equilibrium. The classical formula of the entropy flow is replaced [28] by

$$\vec{J}_s = \frac{1}{T}\left(\vec{J}_q - \boldsymbol{J}_\xi\vec{\xi}\right). \tag{1.4}$$

Here $\boldsymbol{J}_\xi$ is the current density of the transport of the dynamic variable.

The actual form of the entropy production or better of the energy dissipation function reads

$$T\sigma_s = -\frac{1}{T}\operatorname{grad}T\cdot\left(\vec{J}_q - \boldsymbol{J}_\xi\vec{\xi}\right) - \vec{\xi}\cdot\vec{\sigma}_\xi + (\boldsymbol{t} - \boldsymbol{t}^e) : \mathring{\boldsymbol{d}} - \boldsymbol{J}_\xi : \operatorname{Grad}\vec{\xi} \tag{1.5}$$

Here the abbreviating notations

$$\begin{aligned}\boldsymbol{t}^e &= -T\rho\frac{\partial s}{\partial \boldsymbol{d}}\\ \vec{\sigma}_\xi &= \rho\,\mathring{\vec{\xi}} + \operatorname{Div}\boldsymbol{J}_\xi\end{aligned}$$

have been introduced. The function $\boldsymbol{t}^e$ is the equilibrium stress belonging to the present specific entropy and deformation and $\vec{\sigma}_\xi$ is the source density of quantity $\vec{\xi}$.

The four terms in the above formula give account on the entropy generation of four processes. The first term belongs to heat conduction, the second to the relaxation of the dynamic variable, the third to the viscous effects, and the forth to the transport of the dynamic degree of freedom.

The conditions of an equilibrium can be taken from here. According to the first term the temperature has to be uniform, according to the second the dynamic structure has to be relaxed. The third term gives the expression for the stress at an equilibrium. Introducing the notation makes its meaning clear. The last term says that no gradient of $\vec{\xi}$ can be present at an equilibrium.

## 2. Constitutive equations

The first two terms belong vectorial phenomena while the last two to tensorial ones. The Onsager equations fall into two uncoupled set of equations. One for the vectorial phenomena

$$\left(\vec{J}_q - \boldsymbol{J}_\xi \vec{\xi}\right) = -L_{qq}\frac{1}{T}\,\mathrm{grad}\,T - L_{q\xi}\vec{\xi} \tag{2.1}$$

$$\vec{\sigma}_\xi = -L_{\xi q}\frac{1}{T}\,\mathrm{grad}\,T - L_{\xi\xi}\vec{\xi} \tag{2.2}$$

and one for the tensorial quantities

$$\begin{aligned} \boldsymbol{t} - \boldsymbol{t}^e &= \boldsymbol{L}_{dd}\mathring{\boldsymbol{d}} - \boldsymbol{L}_{d\xi}\,\mathrm{Grad}\,\vec{\xi} \\ \boldsymbol{J}_\xi &= \boldsymbol{L}_{\xi d}\mathring{\boldsymbol{d}} - \boldsymbol{L}_{\xi\xi}\,\mathrm{Grad}\,\vec{\xi}. \end{aligned} \tag{2.3}$$

Here the quantities $\boldsymbol{L}_{...}$ are isotropic forth order tensors, the general form of which [29] makes possible to split the set of equations (2.3) into three uncoupled sets, one for the traces

$$\begin{aligned} (p^e - p) &= L^0_{dd}\,\mathrm{div}\,\vec{v} - L^0_{d\xi}\,\mathrm{div}\,\vec{\xi} \\ \mathrm{tr}\,\boldsymbol{J}_\xi &= L^0_{\xi d}\,\mathrm{div}\,\vec{v} - L^0_{\xi\xi}\,\mathrm{div}\,\vec{\xi}, \end{aligned} \tag{2.4}$$

one for the deviatoric parts

$$\begin{aligned} \left(\boldsymbol{t}^D - \boldsymbol{t}^{eD}\right) &= L^D_{dd}\mathring{\boldsymbol{d}} - L^D_{d\xi}\left(\mathrm{Grad}\,\vec{\xi}\right)^D \\ \boldsymbol{J}^D_\xi &= L^D_{\xi d}\mathring{\boldsymbol{d}} - L^D_{\xi\xi}\left(\mathrm{Grad}\,\vec{\xi}\right)^D, \end{aligned} \tag{2.5}$$

and one for the skew symmetric parts

$$0 = L^A_{d\xi}\left(\mathrm{Grad}\,\vec{\xi}\right)^A \tag{2.6}$$

$$\left(\boldsymbol{J}_\xi\right)^A = -L^A_{\xi\xi}\left(\mathrm{Grad}\,\vec{\xi}\right)^A. \tag{2.7}$$

Here the $L_{\dots}$ coefficients are numbers. The upper indices $^0$, $^D$, and $^A$ refer to the scalar, the deviatoric, and the skew-symmetric parts, respectively. The coefficient $L^A_{d\xi}$ equals obviously zero otherwise the equations would be incompatible.

## 3. Heading an engineering application.

Aiming the problem of the disintegration of the wall in some tunnels, some simplifying assumptions are practicable. First of all, the displacements are assumed small and the viscous effects are neglected. Combining equations $(2.4)_2$, $(2.5)_2$, and (2.7),

$$\boldsymbol{J}_\xi = -\frac{1}{3}L^0_{\xi\xi}\,\mathrm{div}\,\xi\boldsymbol{\delta} - L^D_{\xi\xi}(\mathrm{Grad}\,\xi)^D - L^A_{\xi\xi}(\mathrm{Grad}\,\xi)^A \tag{3.1}$$

results for the current density of the transport of the dynamic variable. Its divergence reads

$$\mathrm{Div}\,\boldsymbol{J}_\xi = -\left(\frac{1}{3}L^0_{\xi\xi} + \frac{1}{2}L^D_{\xi\xi} + \frac{1}{2}L^A_{\xi\xi}\right)\Delta\vec{\xi} - \frac{1}{2}\left(L^D_{\xi\xi} - L^A_{\xi\xi}\right)\mathrm{grad}\,\mathrm{div}\,\vec{\xi}. \tag{3.2}$$

Introducing it into the equation (2.2) yields

$$\rho\frac{\partial\vec{\xi}}{\partial t} + L_{\xi\xi}\vec{\xi} = -L_{\xi q}\frac{1}{T}\,\mathrm{grad}\,T + A\Delta\vec{\xi} + B\,\mathrm{grad}\,\mathrm{div}\,\vec{\xi}, \tag{3.3}$$

where the abbreviating notations

$$A = \left(\frac{1}{3}L^0_{\xi\xi} + \frac{1}{2}L^D_{\xi\xi} + \frac{1}{2}L^A_{\xi\xi}\right); \qquad B = \frac{1}{2}\left(L^D_{\xi\xi} - L^A_{\xi\xi}\right) \tag{3.4}$$

have been introduced.

The wall of a tunnel may be approximated sufficiently well with a half space. The above equation falls to one dimensional. Supposing that all the functions depends only on the coordinate perpendicular to the wall, equations (3.3) turn to

$$\rho\frac{\partial\xi_\perp}{\partial t} + L_{\xi\xi}\xi_\perp = -L_{\xi q}\frac{1}{T}\frac{\partial T}{\partial x} + (A+B)\frac{\partial^2\xi_\perp}{\partial x^2} \tag{3.5}$$

$$\rho\frac{\partial\vec{\xi}_\parallel}{\partial t} + L_{\xi\xi}\vec{\xi}_\parallel = A\frac{\partial^2\vec{\xi}_\parallel}{\partial x^2}, \tag{3.6}$$

where $\xi_\perp$ refers to the component of $\vec{\xi}$ perpendicular to the wall and $\vec{\xi}_\parallel$ to the parallel component. The quantity $x$ stands for a Cartesian coordinate perpendicular to the wall. Equation (3.6) shows that only the perpendicular component can be excited.

Turn attention to the stress. Equation $(2.3)_1$—having dropped the viscosity—can be cast to the familiar formula

$$\boldsymbol{t} - \boldsymbol{t}^e = 2\mu^* \boldsymbol{\varepsilon}^* + \lambda^* \Theta^* \boldsymbol{\delta}. \tag{3.7}$$

For the sake of analogy, the symbols

$$\boldsymbol{\varepsilon}^* = \frac{1}{2}\left[\operatorname{Grad}\vec{\varepsilon} + (\operatorname{Grad}\vec{\varepsilon})^T\right] \tag{3.8}$$

$$\Theta^* = \operatorname{div}\vec{\xi} \tag{3.9}$$

$$\mu^* = -\frac{1}{2} L^D_{d\xi} \tag{3.10}$$

$$\lambda^* = \frac{1}{3} L^D_{d\xi} - L^0_{d\xi} \tag{3.11}$$

have been introduced. The symbol $\boldsymbol{\delta}$ is the unit tensor. Equation (3.7) for the one dimensional problem in matrix notation reads

$$\boldsymbol{t} - \boldsymbol{t}^e = 2\mu^* \frac{\partial \xi_\perp}{\partial x} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \lambda^* \frac{\partial \xi_\perp}{\partial x} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{3.12}$$

Accepting the classical formula of linear thermoelasticity

$$\boldsymbol{t}^e = 2\mu \boldsymbol{\varepsilon} + \left[\lambda\Theta - (2\mu + 3\lambda)\alpha(T - T_0)\right] \boldsymbol{\delta}, \tag{3.13}$$

the equilibrium stress functions in matrix form is

$$\boldsymbol{t}^e = 2\mu \frac{\partial u}{\partial x} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \left[\lambda \frac{\partial u}{\partial x} - (2\mu + 3\lambda)\alpha(T - T_0)\right] \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{3.14}$$

where $\lambda$ and $\mu$ are the Lame coefficients, $\alpha$ the coefficient of linear thermal expansion, and $u$ is the displacement of the material perpendicular to the wall.

Cauchy's equation of motion—($\operatorname{Div} t = 0$)—reads

$$(2\mu + \lambda)\frac{\partial^2 u}{\partial x^2} + (2\mu^* + \lambda^*)\frac{\partial^2 \xi_\perp}{\partial x^2} - (2\mu + 3\lambda)\alpha \frac{\partial T}{\partial x} = 0 \tag{3.15}$$

Assuming that no displacement or dynamic degree of freedom are present deep in the rock, a first integration results

$$(2\mu + \lambda)\frac{\partial u}{\partial x} + (2\mu^* + \lambda^*)\frac{\partial \xi_\perp}{\partial x} - (2\mu + 3\lambda)\alpha(T - T_0) = 0 \tag{3.16}$$

For a damage, the deviatoric part of the stress tensor is responsible.

$$\boldsymbol{t}^D = \frac{2}{3}\left(2\mu \frac{\partial u}{\partial x} + 2\mu^* \frac{\partial \xi_\perp}{\partial x}\right) \begin{bmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \tag{3.17}$$

At first sight it seems as if the equations were the same as in the classical theory but the similarity of the equations is only formal. Equation

(3.16) serves to determine the displacement while $\xi_\perp$ has to be known from solving equation (3.5)

Eliminating $u$ from equation (3.17) with equation (3.16),

$$\boldsymbol{t}^D = \frac{4}{3(2\mu+\lambda)}\mathcal{D}\begin{bmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \tag{3.18}$$

with

$$\mathcal{D} = \mu(2\mu + 3\lambda)\alpha(T - T_0) + (\mu^*\lambda - \mu\lambda^*)\frac{\partial \xi}{\partial x} \tag{3.19}$$

results.

## 4. Discussion

The last equation reduces to the classical result if $\mu^*$ and $\lambda^*$ are zero. This case the thermal stress depends only on the difference of the temperatures at the spot and deep in the rock. A thin layer of coat can delay the damage but does not hinder. Equation (3.18) reports such an effect. For a rough estimate, drop the first term on the left hand side of equation (3.5) and the last term on the right hand side and substitute $\xi_\perp$ into the equation.

$$\mathcal{D} = \mu(2\mu + 3\lambda)\alpha(T - T_0) + (\mu\lambda^* - \mu^*\lambda)\frac{L_{\xi q}}{T L_{\xi\xi}}\frac{\partial^2 T}{\partial x^2} \tag{4.1}$$

To judge the practical merit of the theory sketched above is far beyond the possibilities and the authenticity of a thermodynamicist. So I present the idea for further consideration to researchers more familiar with the original problem. But if inclining to reject first consider that, in contrast to Lame's coefficients, thermodynamics do not restrict the magnitudes of $\mu^*$ and $\lambda^*$.

## References

[1] K. Hutter. The foundations of thermodynamics, its basic postulates and implications. *Acta Mechanica, Wien*, 27:1–54, 1977.
[2] L. Onsager. Reciprocal relations in irreversible processes. I. *Phys. Rev.*, 37:405–426, 1931.
[3] L. Onsager. Reciprocal relations in irreversible processes. II. *Phys. Rev.*, 38:2265–2279, 1931.
[4] L. Onsager and S. Maclup. Fluctuations and irreversible processes. *Phys. Rev.*, 91:1505–1512, 1953.
[5] S. Machlup and L. Onsager. Fluctuations and irreversible processes. II. Systems with kinetic energy. *Phys. Rev.*, 91:1512–1515, 1953.
[6] S. R. De Groot. *Thermodynamics of Irreversible Processes.* North-Holland Publ. Co., Amsterdam, 1951.
[7] S. R. De Groot and P. Mazur. *Non-Equilibrium Thermodynamics.* North-Holland Publ. Co., Amsterdam, 1962.
[8] I. Prigogine. *Introduction to Thermodynamics of Irreversible Processes.* Interscience, New York, 1961.
[9] I. Gyarmati. *Non-Equilibrium Thermodynamics.* Springer, Berlin, 1970.

[10] I. Gyarmati. On the wave approach of thermodynamics and some problems of non-linear theories. *J. Non-Equilib. Thermodyn.*, 2:233–260, 1977.

[11] D. Jou, J. Casas-Vázques, and G. Lebon. *Extended Irreversible Thermodynamics.* Springer, New York, Berlin, Heidelberg, 1993.

[12] D. Jou, J. Casas-Vázquez, and G. Lebon. Extended irreversible thermodynamics: An overview of recent bibliography. *J. Non-Equilib. Thermodyn.*, 17:383–396, 1992.

[13] I. Müller and T. Ruggeri. *Extended Thermodynamics.* Springer, Berlin, New York, 1993. Second edition: Rational Extended Thermodynamics. 1998.

[14] L. S. Garcia-Colin and F. J. Uribe. Extended irreversible thermodynamics beyond the linear regime. A critical overview. *J. Non-Equilib. Thermodyn.*, 16:89–128, 1991.

[15] József Verhás. *Thermodynamics and Rheology.* Akadémiai Kiadó and Kluwer Academic Publishers, Budapest and Dordrecht, 1997.

[16] P. Ván and É. Ruszin. Derivation of the basic equations of MHD from the governing principle of dissipative processes. *Acta Physica Hungarica*, 68:227–239, 1990.

[17] V. Ciancio, M. Dolfin, and P. Ván. Thermodynamic theory of dia- and paramagnetic materials. *J. Appl. Electromagnetics and Mechanics.*, 7:237–247, 1996.

[18] S. Holló and B. Nyíri. Equation for cathodic glow sheath. *Acta Physica Hungarica.*, 72:71–88, 1992.

[19] B. Nyíri. Non-equilibrium thermodynamical discussion of ionization in breakdown and glow. In *Fifth International Symposium on the Science and Technology of Light Sources*, page 61, York, 1989.

[20] G. A. Kluitenberg and V. Ciancio. The stress-strain-temperature relation for anisotropic Kelvin-Voigt media. *Atti Acad. di Sci. Lett.*, XL, s.4, f.2, p.1:107–122, 1981.

[21] E. Turrisi, V. Ciancio, and G. A. Kluitenberg. On the propagation of linear transverse acoustic waves... II. some cases of special interest (Poynting-Thomson, Jeffrey, Maxwell, Kelvin-Voigt, Hooke and Newton media). *Physica A*, 116:594–603, 1982.

[22] M. Dolfin V. Ciancio and P. Ván. Thermodynamic theory of dia- and paramagnetic materials. *International Journal of Applied Electromagnetics and Mechanics*, 7:237–247, 1996.

[23] W. Muschik, H. Ehrentraut, and C. Papenfuß. The connection between Ericksen-Leslie equations and the balances of mesoscopic theory of liquid crystals. *Mol. Cryst. Liq. Cryst.*, 262:417–423, 1995.

[24] P. Ván, C. Papenfuss, and W. Muschik. Mesoscopic dynamics of microcracks. *Phys. Rev. E*, 62(5):6206–6215, 2000.

[25] P. Ván. Weakly nonlocal irreversible thermodynamics—the Ginzburg–Landau equation. *Technische Mechanik*, 22(2):104–110, 2002. (cond-mat/0111307).

[26] C. Papenfuss, P. Ván, and W. Muschik. Mesoscopic theory of microcracks. *Archive of Mechanics*, 55(5-6):459–477, 2003. (cond-mat/0212095).

[27] M. Morse. Relation between the critical points of a real function of $n$ independent variables. *Trans. Am. Math. Soc.*, 27:345–396, 1925.

[28] József Verhás. On the entropy current. *Int. J. Non-equilib. Thermodyn.*, 8:201, 1983.

[29] G. F. Smith and R. S. Rivlin. The anisotropic tensors. *Q. Appl. Math.*, 15:308–314, 1957.

Institute of Physics, Budapest University of Technology and Economy. H-1521, Budapest, Hungary
*E-mail address*, J. Verhás: verhas@phy.bme.hu
*URL*: http://newton.phy.bme.hu/~verhas/