

1.3. ELASTIC PROPERTIES

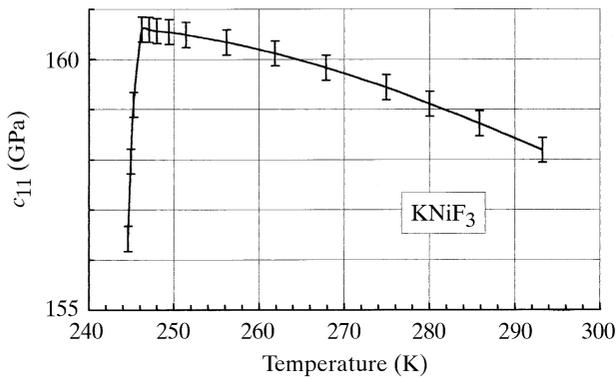


Fig. 1.3.5.4. Temperature dependence of the elastic constant c_{11} in KNiF_3 , which undergoes a para–antiferromagnetic phase transition. Reprinted with permission from *Appl. Phys. Lett.* (Nouet *et al.*, 1972). Copyright (1972) American Institute of Physics.

The softening of c_{44} when the temperature decreases starts more than 100 K before the critical temperature, Θ_c . In contrast, Fig. 1.3.5.4 shows the temperature dependence of c_{11} in KNiF_3 , a crystal that undergoes a para–antiferromagnetic phase transition at 246 K; the coupling between the elastic and the magnetic energy is weak, consequently c_{11} decreases abruptly only a few degrees before the critical temperature. We can generalize this observation and state that the softening of an elastic constant occurs over a large domain of temperature when this constant is the order parameter or is strongly coupled to the order parameter of the transformation; for instance, in the cooperative Jahn–Teller phase transition in DyVO_4 , $(c_{11} - c_{12})/2$ is the soft acoustic phonon mode leading to the phase transition and this parameter anticipates the phase transition 300 K before it occurs (Fig. 1.3.5.5).

1.3.5.3. Pressure dependence of the elastic constants

As mentioned above, anharmonic potentials are needed to explain the stress dependence of the elastic constants of a crystal. Thus, if the strain-energy density is developed in a polynomial in terms of the strain, only the first and the second elastic constants are used in linear elasticity (harmonic potentials), whereas higher-order elastic constants are also needed for nonlinear elasticity (anharmonic potentials).

Concerning the pressure dependence of the elastic constants (nonlinear elastic effect), considerable attention has been paid to their experimental determination since they are a unique source of significant information in many fields:

(i) In *geophysics*, a large part of the knowledge we have on the interior of the earth comes from the measurement of the transit time of elastic bursts propagating in the mantle and in the core (in the upper mantle, the average pressure is estimated to be about a few hundred GPa, a value which is comparable to that of the elastic stiffnesses of many materials).

(ii) In *solid-state physics*, the pressure dependence of the elastic constants gives significant indications concerning the stability of crystals. For example, Fig. 1.3.5.2 shows the pressure dependence of the elastic constants of KZnF_3 , a cubic crystal belonging to the perovskite family. As mentioned previously, this crystal is known to be stable over a wide range of temperature and the elastic stiffnesses c_{ij} depend linearly on pressure. It may be noted that, consequently, the third-order elastic constants

Table 1.3.5.2. Order of magnitude of the temperature dependence of the elastic stiffnesses for different types of crystals

Type of crystal	$(\partial \ln c_{11} / \partial \Theta)_p$ (K^{-1})	$(\partial \ln c_{44} / \partial \Theta)_p$ (K^{-1})
Ionic	-10^{-3}	-3×10^{-4}
Covalent	-10^{-4}	-8×10^{-5}
Metallic	-2×10^{-4}	-3×10^{-4}

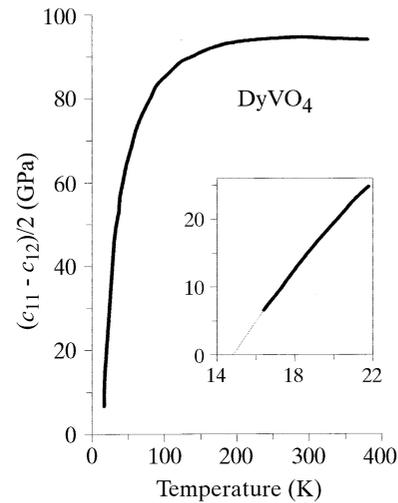


Fig. 1.3.5.5. Temperature dependence of $(c_{11} - c_{12})/2$ in DyVO_4 , which undergoes a cooperative Jahn–Teller phase transition (after Melcher & Scott, 1972).

(TOECs) are constant. On the contrary, we observe in Fig. 1.3.5.6 that the pressure dependence of the elastic constants of TlCdF_3 , a cubic crystal belonging to the same family but which is known to become unstable when the temperature is decreased to 191 K (Fischer, 1982), is nonlinear even at low pressures. In this case, the development of the strain-energy density in terms of strains cannot be stopped after the terms containing the third-order elastic constants; the contributions of the fourth- and fifth-order elastic constants are not negligible.

(iii) For practical use in the case of technical materials such as concrete or worked metals, the pressure dependence of the elastic moduli is also required for examining the effect of applied stresses or of an applied hydrostatic pressure, and for studying residual stresses resulting from loading (heating) and unloading (cooling) the materials.

1.3.6. Nonlinear elasticity

1.3.6.1. Introduction

In a solid body, the relation between the stress tensor T and the strain tensor S is usually described by Hooke's law, which postulates linear relations between the components of T and S (Section 1.3.3.1). Such relations can be summarized by (see equation 1.3.3.2)

$$T_{ij} = c_{ijkl} S_{kl},$$

where the c_{ijkl} 's are the elastic stiffnesses.

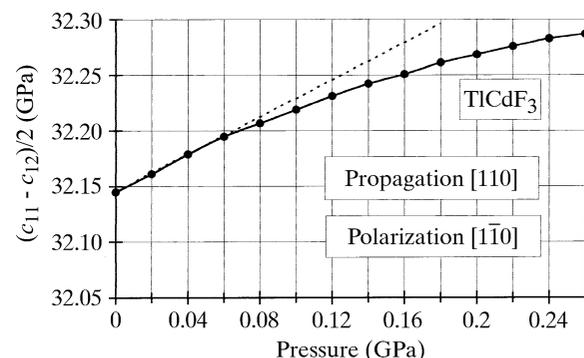


Fig. 1.3.5.6. Pressure dependence of the elastic constants $(c_{11} - c_{12})/2$ in TlCdF_3 . Reproduced with permission from *Ultrasonics Symposium Proc. IEEE* (Fischer *et al.*, 1980). Copyright (1980) IEEE.

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

For a solid under finite strain conditions, Hooke's law, valid for infinitesimal deformations, does not hold, and the fundamental definitions for stress and strain must be revisited.

1.3.6.2. Lagrangian and Eulerian description

Finite elastic strains may be treated from two different viewpoints using either the *Lagrangian (material)* or the *Eulerian (spatial)* descriptions.

Let us consider a fixed rectangular Cartesian coordinate system with axes x_i ($i = 1, 2, 3$). Any particular position vector \mathbf{r} of components (x_1, x_2, x_3) denotes a point in space. A point that always moves with the material is called a particle or *material point*. Let every particle be identified by its coordinates at some reference time t_0 . These reference coordinates, referred to the same Cartesian system, will be denoted by (a_1, a_2, a_3) and the corresponding position vector \mathbf{a} . A particular vector \mathbf{a} can serve as a name for the particle located at that position at the reference time t_0 .

The vectors \mathbf{r} and \mathbf{a} both specify a position in a fixed Cartesian frame of reference. At any time, we associate each \mathbf{r} with an \mathbf{a} by the rule that \mathbf{r} is the present position vector of the particle initially at \mathbf{a} . This connection between \mathbf{r} and \mathbf{a} is written symbolically as

$$\mathbf{r} = \mathbf{r}(t, \mathbf{a}) \quad \text{or} \quad x_i = x_i(t, a_1, a_2, a_3), \quad (1.3.6.1)$$

where

$$\mathbf{a} = \mathbf{r}(t_0, \mathbf{a}) \quad \text{or} \quad a_i = x_i(t_0, a_1, a_2, a_3). \quad (1.3.6.2)$$

The coordinates a_i that identify the particles are called *material coordinates*. A description that, like (1.3.6.1), uses (t, a_1, a_2, a_3) as independent variables is called a *material* or *Lagrangian* description.

The converse of (1.3.6.1) and (1.3.6.2) may be written

$$\mathbf{a} = \mathbf{a}(t, \mathbf{r}) \quad \text{or} \quad a_i = a_i(t, x_1, x_2, x_3), \quad (1.3.6.3)$$

where

$$\mathbf{r} = \mathbf{a}(t_0, \mathbf{r}) \quad \text{or} \quad x_i = a_i(t_0, x_1, x_2, x_3). \quad (1.3.6.4)$$

A spatial description or *Eulerian* description uses the independent variables (t, x_1, x_2, x_3) , the x_i being called *spatial coordinates*.

Now, for the sake of simplicity, we shall work with the Lagrangian formulation exclusively. For more details see, for instance, Thurston (1964) and Wallace (1970, 1972).

1.3.6.3. Strain and stress tensors

The displacement vector from the reference position of a particle to its new position has as components

$$u_i = x_i - a_i. \quad (1.3.6.5)$$

The term strain refers to a change in the relative positions of the material points in a body. Let a final configuration be described in terms of the reference configuration by setting t equal to a constant in (1.3.6.1). Then t no longer appears as a variable and (1.3.6.1) can be written

$$x_i = x_i(a_1, a_2, a_3),$$

where the a_i are the independent variables. It follows that

$$dx_j = \frac{\partial x_j}{\partial a_i} da_i = \left(\frac{\partial u_j}{\partial a_i} + \delta_{ij} \right) da_i. \quad (1.3.6.6)$$

Let now the particle initially at (a_1, a_2, a_3) move to (x_1, x_2, x_3) . The square of the initial distance to a neighbouring particle whose initial coordinates were $a_j + da_j$ is

$$ds^2 = da_j da_j.$$

The square of the final distance to the same neighbouring particle is

$$ds^2 = dx_j dx_j.$$

In a material description, the strain components S_{ik} are defined by the following equations:

$$dx_j dx_j - da_j da_j = 2S_{ik} da_i da_k. \quad (1.3.6.7)$$

Substituting (1.3.6.6) into (1.3.6.7), it follows that

$$\left(\frac{\partial u_j}{\partial a_i} + \delta_{ji} \right) \left(\frac{\partial u_j}{\partial a_k} + \delta_{jk} \right) da_i da_k - da_j da_j = 2S_{ik} da_i da_k.$$

Hence

$$S_{ik} = \frac{1}{2} \left(\frac{\partial u_k}{\partial a_i} + \frac{\partial u_i}{\partial a_k} + \frac{\partial u_j}{\partial a_i} \frac{\partial u_j}{\partial a_k} \right).$$

If the products and squares of the displacement derivatives are neglected, the strain components reduce to the usual form of 'infinitesimal elasticity' [see equation (1.3.1.8)]:

$$S_{ik} = \frac{1}{2} \left(\frac{\partial u_i}{\partial a_k} + \frac{\partial u_k}{\partial a_i} \right).$$

It is often useful to introduce the Jacobian matrix associated with the transformation (\mathbf{a}, \mathbf{x}) . The components of this matrix are

$$J = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{pmatrix},$$

where

$$\alpha_{ik} = \frac{\partial x_i}{\partial a_k} = \frac{\partial u_j}{\partial a_k} + \delta_{jk}.$$

From the definition of matrix J , one has

$$d\mathbf{x} = J d\mathbf{a}$$

and

$$dx^2 - da^2 = (d\mathbf{x})^T d\mathbf{x} - (d\mathbf{a})^T d\mathbf{a} = (d\mathbf{a})^T (J^T J - \delta) d\mathbf{a},$$

where $(d\mathbf{a})^T$, $(d\mathbf{x})^T$ and J^T are the transpose matrices of $d\mathbf{a}$, $d\mathbf{x}$ and J , respectively, and δ is the Kronecker matrix.

The Lagrangian strain matrix S may then be written symbolically:

$$S = \frac{1}{2} (J^T J - \delta). \quad (1.3.6.8)$$

When finite strains are concerned, we have to distinguish three states of the medium: the natural state, the initial state and the final or present state: The *natural* state is a state free of stress. The *initial* state is deduced from the natural state by a homogeneous strain. The *final* state is deduced from the initial state by an arbitrary strain.

Concerning the stress tensor, as pointed out by Thurston (1964), the stress-deformation relation is complicated in nonlinear elasticity because 'the strain is often referred to a natural unstressed state, whereas the stress T_{ij} is defined per unit area of the deformed body'. For this reason, the differential of work done by the stress is not equal to the stress components times the differentials of the corresponding strain components. So, following Truesdell & Toupin (1960), we shall introduce a *thermodynamic tension tensor* t_{ij} defined as the first derivative of the energy with respect to strain. If the internal energy U per unit