International Tables for Crystallography (2006). Vol. D, Section 1.3.5.3, p. 91.

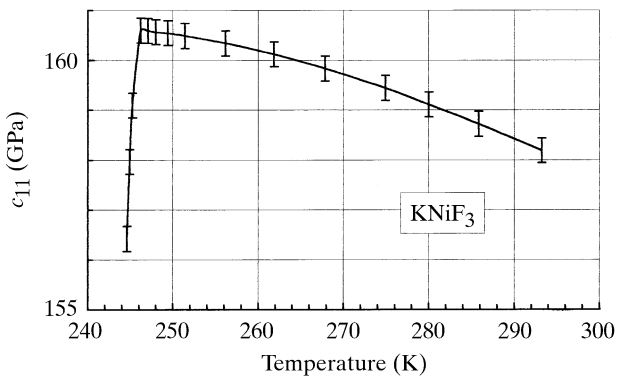

Fig. 1.3.5.4. Temperature dependence of the elastic constant c_{11} in $KNiF_3$, which undergoes a para–antiferromagnetic phase transition. Reprinted with permission from *Appl. Phys. Lett.* (Nouet *et al.*, 1972). Copyright (1972) American Institute of Physics.

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).

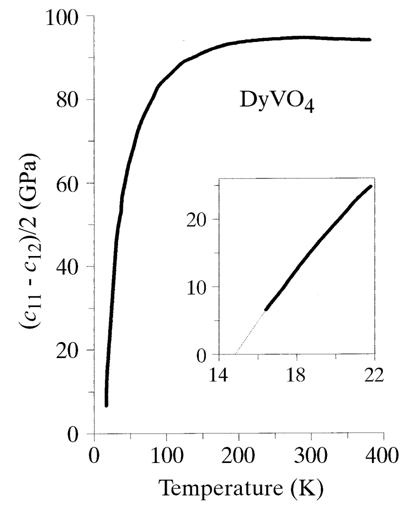

Fig. 1.3.5.5. Temperature dependence of $(c_{11} - c_{12})/2$ in $DyVO_4$, which undergoes a cooperative Jahn–Teller phase transition (after Melcher & Scott, 1972).

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 (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.

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}

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.

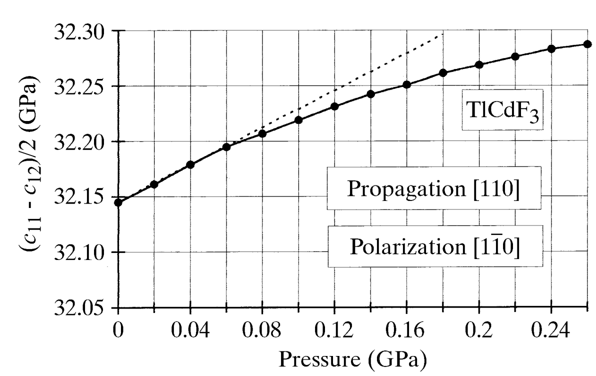

Fig. 1.3.5.6. Pressure dependence of the elastic constants $(c_{11} - c_{12})/2$ in $TlCdF_3$. Reproduced with permission from *Ultrasonics Symposium Proc. IEEE* (Fischer *et al.*, 1980). Copyright (1980) IEEE.

references