Elastic energy - gradient expansion

Energy of a deformed body can not depend on displacement itself because for uniform displacement energy is not changed.

Thus it can depend only on gradients of displacement $\frac{\partial u_i}{\partial x_k}$

One such term in the elastic energy would be

$$\lambda\left(\frac{\partial u_i}{\partial x_i}\right)^2 = \lambda(\mathrm{div}\,\vec{u})^2$$

Another one

$$\sum_{ik}\left(\frac{\partial u_i}{\partial x_k}\right)^2$$

However arbitrary gradients are not allowed because the energy is also invariant with respect to uniform rotations

For rotation on an infinitesimal angle $\delta\Omega$

$$\vec{u} = \delta\vec{\Omega} \times \vec{r}$$

Thus $\delta\vec{\Omega} = \frac{\text{rot}\,\vec{u}}{3}$

Since energy should not depend on $\delta\Omega$ it should not contain $[\text{rot}\,u]^2$ => from the gradient term $\left(\frac{\partial u_i}{\partial x_k}\right)^2$ we should exclude antisymmetric part $\frac{\partial u_i}{\partial x_k} - \frac{\partial u_k}{\partial x_i}$

As a result we arrive to elastic energy

$$F = \int dV \left[\frac{\lambda}{2}(\text{div}\,\vec{u})^2 + \mu (u_{ik})^2 \right]$$

with $u_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right)$

Thermal expansion

Let us consider deformations due to change in the temperature of the body.

At $T = T_0$ body is assumed to be undeformed. If $T \neq T_0$ the body will be deformed even in the absence of external forces.

Thus the free energy will contain also linear terms in u_{ik}.

The only ivariant one can make from u_{ik} is $u_{ii} = \operatorname{div}\vec{u}$

Thus

$$F(T) = F_0(T) - KA(T)u_{ii} + \frac{K}{2}u_{ll}^2 + \mu\left(u_{ik} - \frac{1}{3}\delta_{ik}u_{ll}\right)^2$$

If T is close to T_0 then we can expand $A(T) = \alpha(T-T_0) + \beta(T-T_0)^2 + \ldots$

Keeping only linear term we obtain

$$F(T) = F_0 T - K\alpha(T-T_0)u_{ii} + \frac{K}{2}u_{ll}^2 + \mu\left(u_{ik} - \frac{1}{3}\delta_{ik}u_{ll}\right)^2$$

Using $\sigma_{ik} = \dfrac{\partial F}{\partial u_{ik}}$ we obtain

$$\sigma_{ik} = -K\alpha(T-T_0)\delta_{ik} + K u_{ll}\delta_{ik} + 2\mu\left(u_{ik} - \frac{1}{3}\delta_{ik}u_{ll}\right).$$

In the absence of external forces there can be no internal stresses $\Rightarrow$ $\sigma_{ik} = 0 \Rightarrow$

$u_{ik} \propto \delta_{ik}$ and $u_{ll} = \alpha(T-T_0) \Rightarrow$

- $\dfrac{\delta V}{V} = \alpha(T-T_0) \Rightarrow \alpha$ – thermal expansion coefficient.

If the body is non-uniformly heated in the equation of motion $\dfrac{\partial \sigma_{ik}}{\partial x_k} = 0$

- we should include the term $-K\alpha(T-T_0)\delta_{ik}$ in σ_{ik}. As a result equation from p. 15 reads

$$\frac{3(1-\sigma)}{1+\sigma}\,\mathrm{grad}\,\mathrm{div}\,u - \frac{3(1-2\sigma)}{2(1+\sigma)}\,\mathrm{rot}\,\mathrm{rot}\,u = \alpha\nabla T$$

Elasticity of crystals

In general

$$F = \frac{1}{2}\lambda_{iklm} u_{ik} u_{lm}, \quad \sigma_{ik} = \lambda_{iklm} u_{lm}$$

elastic modulus tensor

Since $u_{ik} = u_{ki} \Rightarrow$

- $\lambda_{iklm} = \lambda_{kilm} = \lambda_{ikml} = \lambda_{lmik}$

For the isotropic body we should construct λ_{iklm} out of δ_{jn}

The only two tensors satisfying symmetry relations are $\delta_{ik}\delta_{lm}$ and $\delta_{il}\delta_{km} + \delta_{im}\delta_{kl}$

- Thus $\lambda_{iklm} = \lambda\delta_{ik}\delta_{lm} + \mu(\delta_{il}\delta_{km} + \delta_{im}\delta_{kl})$

and $F_{el} = \frac{1}{2}\int dV\left[\lambda u_{ll}^2 + 2\mu u_{ik} u_{ik}\right]$

In general there are 21 independent components of λ_{iklm}. To see it, note, that there are only six independent combinations of ik and lm. These are denoted by

$1 = xx$, $2 = yy$, $3 = zz$, $4 = yz$, $5 = xz$, $6 = xy$

Then we can use $C_{\alpha\beta}$ instead of λ_{iklm} with $\alpha, \beta = 1, 2, \dots 6$

For $\alpha = 1$ β can be any of 6 numbers

But since $C_{\alpha\beta} = C_{\beta\alpha}$ then $C_{12} = C_{21}$ and

for $\alpha = 2$ β is $2, 3 \dots 6$ (5 number)

for $\alpha = 3$ β is $3, 4, 5, 6$ etc.

As a result we have

$6 + 5 + 4 + 3 + 2 + 1 = 21$ independent components

Depending on crystal symmetry, number of components can be reduced.

Tetragonal system

λ_{iklm} transforms as $x_i x_k x_l x_m$

Because of reflection symmetry

- $x \to -x$, $y \to y$, $z \to z$ and

  $x \to x$, $y \to -y$, $z \to z$

all components with an odd number of like indices vanish.

Further more, a 90° rotation leads to

- $x \to y$, $y \to -x$, $z = z \Rightarrow$

$\lambda_{xxxx} = \lambda_{yyyy}$; $\lambda_{xxzz} = \lambda_{yyzz}$, $\lambda_{xzxz} = \lambda_{yzyz}$

As a result there are 6 elastic constants

$$F = \frac{1}{2} \lambda_{xxxx} (u_{xx}^2 + u_{yy}^2) + \frac{1}{2} \lambda_{zzzz} u_{zz}^2 +$$

$$+ \lambda_{xxzz} (u_{xx} u_{zz} + u_{yy} u_{zz}) + \lambda_{xxyy} u_{xx} u_{yy} +$$

$$+ 2 \lambda_{xyxy} u_{xy}^2 + 2 \lambda_{xzxz} (u_{xz}^2 + u_{yz}^2)$$

For the <u>Cubic system</u>

x, y and z are equivalent $\Rightarrow$

$\lambda_{xxxx} = \lambda_{zzzz}$, $\lambda_{xxzz} = \lambda_{xxyy}$

$\lambda_{xyxy} = \lambda_{xzxz}$

and one has 3 independent elastic constants.

- $$F = \frac{1}{2}\lambda_{xxxx}(u_{xx}^2 + u_{yy}^2 + u_{zz}^2) + \lambda_{xxyy}(u_{xx}u_{yy} + u_{xx}u_{zz} + u_{yy}u_{zz}) + 2\lambda_{xyxy}(u_{xy}^2 + u_{xz}^2 + u_{yz}^2)$$

In general the number of modulus is

Triclinic		21
Monoclinic	C_2, C_s, C_h	13
Orthorombic	D_2, C_{2v}, C_{2h}	9
Tetragonal	C_4, S_4, C_{4h}, C_{4v}, D_{2d}, D_4, D_{4h}	6
Hexagonal		5
Cubic		3

Thermal expansion of crystals

$$u_{ik} = \frac{1}{3}\alpha_{ik}(T - T_0)$$

α_{ik} is symmetric tensor

It has 3 components for triclinic, monoclinic and orthorombic,

2 components for tetragonal and hexagonal

and 1 component for cubic lattice.