BULLETIN OF THE POLISH ACADEMY OF SCIENCES
TECHNICAL SCIENCES
Vol. 52, No. 2, 2004

One-dimensional elongation of a cubic crystal

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Abstract. Large elongation in one definite direction of a crystal of cubic symmetry is considered. The equations of second order elasticity theory are applied. In this approximation three constants of the second order and six constants of the third order characterize the crystal. The stress is a function of the elongation direction. The elongation directions for which the stress reaches an extreme value have been analyzed.

Keywords: cubic crystal, elongation, material nonlinearity.

1. Second order elasticity

Crystals are of special interest in a fundamental research. Plates or bars cut out from a crystal are frequently used in physical equipment. Taking into account the symmetries (called point groups) the crystals may be divided into 32 classes. All crystals belonging to one class have the same macroscopic symmetry. Cubic crystals posses the highest crystallographic symmetry. In the linear case their mechanical behaviour is described by three elastic constants. Triclinic crystals belong to the class of the lowest symmetry. In the linear case triclinic crystals are described by twenty-one elastic constants.

Clusters of chaotically oriented single crystals are globally isotropic. Isotropic material posseses the highest mathematically possible symmetry. Mechanical properties of linear isotropic material are described by only two elastic constants. Most of the experience in engineering is connected with isotropic materials. It must be stressed that mechanically isotropic crystals do not exist.

External load applied to a crystal results in its deformation. Since the crystal is not isotropic the deformation of a crystal essentially differs from that of isotropic material. In the presented paper the analysis of the forces, necessary to produce a defined in advance elongation is given. We confine to one symmetry only, namely to the cubic symmetry. Typical material of this symmetry is the crystal of copper or silver. Obviously linear material is of special interest. However in the nonlinearity some additional, very important phenomena are present. Trying to avoid complex, non-transparent considerations we do not consider general elasticity, but confine to the second-order theory. The second order theory of elasticity was presented in the monograph of Green and Adkins [1]. All equations of the first chapter of the presented paper are based on this monography. Introduce the Cartesian coordinates x_j. The material point of the body is identified by its position x_j in the stress-free initial state. In the course of time the point x_j moves to a new position. The values of the displacement vector u_i are functions of the Cartesian coordinates x_j and time t, $u_i = u_i(x_j, t)$. In the presented paper we compare the initial and final states and time t serves only as parameter. Therefore for simplicity we shall write $u_i = u_i(x_j)$. Partial derivative of $u_i(x_j)$ with respect to x_j is the displacement gradient $u_{i,j}$. The strain tensor ε_{ij} may be expressed by the displacement gradient

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,i} + u_{j,i} + u_{r,i}u_{r,j}). \tag{1}$$

Summation convention is accepted in the whole presented paper. Due to the presence of the product $u_{r,i}u_{r,j}$ the deformation tensor ε_{ij} always is a nonlinear function of the displacement gradient. The linear measure of strain which disregards the nonlinear term may be used only in the linear theory, where the stress is a linear function of strain. The relation (1) is purely geometrical. No material properties are involved. The elastic energy Φ (strain energy) is a nonlinear function of strain ε_{ij}.

In second order elasticity the expression for the elastic energy Φ (per unit volume in the stress-free state) takes into account the squares, but neglects the cubes and higher powers of strain tensor ε_{ij}. The elastic energy Φ reads

$$\Phi = \frac{1}{2}c_{ijpq}\varepsilon_{ij}\varepsilon_{pq} + \frac{1}{6}c_{ijpqrs}\varepsilon_{ij}\varepsilon_{pq}\varepsilon_{rs}. \tag{2}$$

The elastic energy is a polynomial of the third grade of strain, but polynomial of the sixth grade of the displacement gradient. The coefficients 1/2 and 1/6 present in Eq. (2) are commonly accepted in the literature [2].

The fourth rank tensor c_{ijpq} is the tensor of second order elastic constants and c_{ijpqrs} is the tensor of third order elastic constants. In some older papers those tensors are called first and second order elastic constants, respectively. Since the expression (2) is homogeneous in ε_{ij} it may be assumed that $c_{ijpq} = c_{pqij}$ and $c_{ijpqrs} = c_{pqijrs} = c_{ijrspq}$. Since ε_{ij} is symmetric without loosing the generality it may be assumed that the constants satisfy the relations $c_{ijpq} = c_{jipq}$ and $c_{ijpqrs} = c_{jipqrs}$. The elastic constants of the second order and of the third order may therefore be assumed to possess the following symmetries

$$c_{ijpq} = c_{pqij} = c_{jipq}, \tag{3}$$

$$c_{ijpqrs} = c_{pqijrs} = c_{ijrspq} = c_{jipqrs}. \tag{4}$$

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Symmetry of the crystal results in additional symmetries. As mentioned above the second order elastic constants c_{ijpq} for triclinic symmetry may be expressed by 21 different material constants. In the simplest case of cubic symmetry there are only 3 non-zero different constants of the second order and 6 material constants of the third order. The 81 constants c_{ijkm} and 729 constants c_{ijkmpq} may therefore for the cubic crystal be expressed by only 9 elastic constants. The isotropic material is characterized by 2 constants of second order (Lame constants) and 3 constants of third order only. There exist several different methods of measuring the constants of the third order. A measurement of forces in static deformation is one of them, but the most frequently used method is based on measurements of the ultrasonic wave speeds.

Denote by H_{ij} the symmetrized derivative of the elastic energy Φ with respect to the deformation ε_{ij}

$$H_{ij} = \frac{\partial \Phi}{\partial \varepsilon_{ij}} + \frac{\partial \Phi}{\partial \varepsilon_{ji}}. \tag{5}$$

From (2) and the symmetries (3)–(4) there follows

$$\frac{\partial \Phi}{\partial \varepsilon_{ij}} = c_{ijpq}\varepsilon_{pq} + \frac{1}{2}c_{ijpqrs}\varepsilon_{pq}\varepsilon_{rs} \tag{6}$$

and further

$$H_{ij} = 2c_{ijpq}\varepsilon_{pq} + c_{ijpqrs}\varepsilon_{pq}\varepsilon_{rs}. \tag{7}$$

The stress tensor τ_{ij} may be expressed by the function H_{ij} and the displacement gradient $u_{i,j}$

$$2\tau_{ij} = H_{ij} + H_{ir}u_{j,r} \tag{8}$$

The stress tensor τ_{ij} is not symmetric. It is in fact the first Piola-Kirchhoff stress tensor [3]. This tensor may be expressed by the deformation gradient and material constants.

Consider elongation in the direction n_i. This is a homogeneous deformation in which material elements parallel to n_i increase their length, and the material elements orthogonal to n_i remain unchanged. The displacement vector u_i is parallel to n_i and its length is proportional to the distance $n_r x_r$ from the plane $n_r x_r = 0$. Therefore the displacement u_i reads

$$u_i(x_r) = \nu n_i n_r x_r, \tag{9}$$

where ν is the measure of deformation. On the whole plane $n_r x_r = \text{const}$ the displacement vector is the same. The displacement gradient $u_{i,j}$ and the strain tensor ε_{ij} may now be calculated from (1) and (9)

$$u_{i,j} = \nu n_i n_j, \ \varepsilon_{ij} = \nu n_i n_j + \frac{1}{2}\nu^2 n_i n_j. \tag{10}$$

For each material, linear and nonlinear strain tensor consists of a term proportional to ν and a term proportional to ν^2. Substitute the above expression into (8) and take into account the symmetries of c_{ijpq} and c_{ijpqrs} to obtain the following expression for the stress tensor

$$\tau_{ij} = \nu c_{ijpq}n_p n_q + \nu^2\left(\frac{1}{2}c_{ijpqrs}n_p n_q n_r n_s + \frac{1}{2}c_{ijpq}n_p n_q + n_j c_{irpq}n_r n_p n_q\right) \tag{11}$$

The stress tensor τ_{ij} is determined uniquely by the strain energy Φ and the shear. In (11) the terms of the order ν^3 have been neglected.

The stress vector τ_i acting on a surface with unit normal n_i equals to the product of the stress tensor τ_{ij} and the vector n_i

$$t_j = \tau_{ij}n_i. \tag{12}$$

In the presented Section we do not consider the stresses acting on other surfaces. From the above relations there follows

$$t_j = \nu c_{ijpq}n_i n_p n_q + \nu^2\left(\frac{1}{2}c_{ijpqrs}n_i n_p n_q n_r n_s + \frac{1}{2}c_{ijpq}n_i n_p n_q + n_j c_{irpq}n_i n_r n_p n_q\right) \tag{13}$$

In general this vector is not collinear with n_i. Its squared length equals to $t_i t_i$ and its projection on n_i equals to $t_i n_i$. It follows that the modulus of the component s_n parallel to n_i and the modulus of the component s_t orthogonal to n_i are given by the relations

$$\begin{aligned} s_n &= t_j n_j, \\ s_t^2 &= t_j t_j - s_n^2. \end{aligned} \tag{14}$$

Obviously s_n and s_t may be calculated within ν^2, not ν^3. In accordance with (13) the formulae of the form

$$\begin{aligned} s_n &= \nu s_{n1} + \nu^2(s_{n2} + s_{n3}), \\ s_t &= n s_{t1} + n^2(s_{t2} + s_{t3}) \end{aligned} \tag{15}$$

are expected. From (13–14) the expressions for s_{n1}, s_{n2}, s_{n3} follow

$$\begin{aligned} s_{n1} &= c_{ijpq}n_i n_j n_p n_q, \\ s_{n2} &= \frac{3}{2}c_{ijpq}n_i n_j n_p n_q, \\ s_{n3} &= \frac{1}{2}c_{ijpqrs}n_i n_j n_p n_r n_q n_s. \end{aligned} \tag{16}$$

Pass to the calculation of s_t. The form (16) must be valid for each choice of c_{ijpq}, c_{ijpqrs} and ν. The long formulae for s_{t1}, s_{t2} and s_{t3} will not be quoted. The component s_t may be computed from (14).

The inclination angle ξ of the stress to the surface, i.e. the angle between t_j and n_j is of a great interest. Obviously there is

$$\cos\xi = \frac{|t_j n_j|}{\sqrt{t_j t_j}}, \quad \operatorname{tg}\xi = \frac{t_t}{t_n}. \tag{17}$$

Stiffness s equals to the ratio of the component of t_j in the direction n_j and the measure of deformation ν. The sum s_n, cf. (16) is the measure of stiffness.

Since the expressions (17) for s_{n1}, s_{n2} and s_{n3} are even functions of n_i the values s_{n1}, s_{n2} and s_{n3} are invariant under the transformation

$$(n_1, n_2, n_3) \Rightarrow (-n_1, -n_2, -n_3). \tag{18}$$

Note that the vector t_j as given by (13) is an odd function of n_i. Therefore its length is an even function of n_i. It follows that $t_j t_j$ and s_t are invariant under the transformation (18). More detailed examination of the expressions proves that for cubic symmetry the six above values are additionally invariant under the transformations

$$(n_1, n_2, n_3) \Rightarrow (n_2, n_1, n_3), (n_1, n_2, n_3) \Rightarrow (n_1, n_3, n_2), (n_1, n_2, n_3) \Rightarrow (n_3, n_2, n_1). \quad (19)$$

The above invariances allow to confine the analysis to the directions located between the vectors (1,0,0), (1,1,0) and (1,1,1), cf. Fig. 1.

2. Linear elasticity

Linear elastic properties of a cubic crystal are defined by three independent elastic constants of second order. In the abbreviated notation ($\varepsilon_1 = \varepsilon_{11}, \varepsilon_2 = \varepsilon_{22}, ..., \varepsilon_4 = 2\varepsilon_{23}$, etc.) they are h_{11}, h_{12} and h_{44}, cf. [2]. All 81 components of the elastic constants of tensor c_{ijpq} may be expressed by the three constants of the h_{11}, h_{12} and h_{44}, namely

$$\begin{aligned} &c_{1111} = c_{2222} = c_{3333} = h_{11}, \\ &c_{1122} = c_{1133} = c_{2233} = c_{2211} = c_{3311} = c_{3322} = h_{12}, \quad (20) \\ &c_{2323} = c_{2332} = c_{3223} = ... = c_{1212} = c_{1221} = h_{44}. \end{aligned}$$

All other components of the tensor c_{ijpq} e.g. c_{1112} are equal to zero.

To gain recognition of the stresses in this Section we shall analyze the influence of elastic constants on stress in pure one-dimensional strain. We assume in turn: i) $h_{11} = 1$, $h_{12} = 0$, $h_{44} = 0$, ii) $h_{11} = 0$, $h_{12} = 1$, $h_{44} = 0$ and iii) $h_{11} = 0$, $h_{12} = 0$, $h_{44} = 1$. As an example a definite material (copper) will be considered later.

Calculate the stresses for the following eight selected directions

$$\begin{aligned} &n_i^{(1)} = (0,0,1), \quad n_i^{(2)} = (1/2,0,1), \quad n_i^{(3)} = (0,1,1), \\ &n_i^{(4)} = (1,1/2,1), \quad n_i^{(5)} = (1,1,1), \quad n_i^{(6)} = (1/3,1/3,1), \\ &n_i^{(7)} = (2/3,1/3,1), \quad n_i^{(8)} = (2/3,2/3,1). \quad (21) \end{aligned}$$

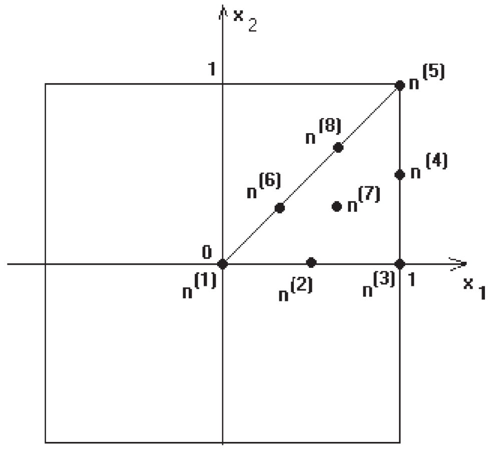

Fig. 1. Projection of selected directions on the $x_3 = 0$ surface

In Fig. 1 the front side of a cube of dimension $2 \times 2 \times 2$ is shown. This side is a square of dimension 2×2, situated on the plane $x_3 = 1$. In Fig. 1 there are shown the points, where the eight vectors $n_i^{(1)}, n_i^{(2)}, ..., n_i^{(8)}$ intersect the plane $x_3 = 1$. The three vectors $n_i^{(1)}$, $n_i^{(3)}$, $n_i^{(5)}$ are the symmetry directions of the cube. Due to the symmetry of the problem (cf. Eq. (19)) each extension of the crystal (defined by vector n_i) is equivalent to an extension situated in the triangle (n_1, n_3, n_5). In particular the extensions in the directions (1,1,1/2) and (1/2,1,1) are equivalent to the extension in the direction (1,1/2,1) listed above. Detailed calculations show, that the spherical angle corresponding to the triangle $n_i^{(1)}, n_i^{(3)}, n_i^{(5)}$ equals to $\pi/12$. This angle is equal to 1/48 of full spherical angle 4π, that represents all possible directions of the three dimensional space. Note that for an isotropic material all extension directions are equivalent to only one, arbitrary chosen direction.

For the eight directions (21) the linear stress is determined by values listed in Table 1. The normal linear stress t_{n1} and the linear shear stress t_{t1} are given. The angle ξ is the inclination of the total stress to the surface. The values 1.571 marked by an asterisk are the limit values, where the expression for tangens has the form 0/0.

Table 1
Longitudinal and transverse components of linear stress and ξ

	$h_{11} = 1$			$h_{12} = 1$			$h_{44} = 1$		
	t_{n1}	t_{t1}	ξ	t_{n1}	t_{t1}	ξ	t_{n1}	t_{t1}	ξ
$n_i^{(1)}$	1.000	0	0	0	0	1.571*	0	0	1.571*
$n_i^{(2)}$	.680	.240	.339	0.320	0.240	.644	.640	.480	.644
$n_i^{(3)}$	.500	0	0	.500	0	0	1.000	0	0
$n_i^{(4)}$	.407	.106	.252	.593	.105	.175	1.185	.210	.175
$n_i^{(5)}$	.333	0	0	.667	0	0	1.333	0	0
$n_i^{(6)}$	.686	.281	.388	.314	.281	.729	.628	.561	.729
$n_i^{(7)}$	.500	.198	.388	.500	.198	.378	1.000	.397	.378
$n_i^{(8)}$	.391	.147	.359	.609	.147	.237	1.218	.294	.237

The actual values of stress t_{n1} and t_{t1} may be obtained by multiplying the values quoted in the Table by the value of the elastic constant of the material (h_{11}, h_{12}, or h_{44}) and the deformation measure ν. Note that $n_i^{(1)}$, $n_i^{(3)}$, $n_i^{(5)}$ are the symmetry directions of the cube and therefore the stress is parallel to the elongation direction.

The overall (linear) properties take into account the actual values of all elastic constants of the second order. Calculate the stresses for one definite material, namely to copper. Copper crystallizes in the cubic symmetry of the type VIIb for which there exist only three different elastic constants of second order h_{11}, h_{12}, h_{44} and six different elastic constants of the third order h_{111}, h_{112}, h_{123}, h_{144}, h_{155}, h_{456}, cf. [2, 4]

$$h_{11} = 169 \text{ GPa}, \; h_{12} = 122 \text{ GPa}, \; h_{44} = 73.5 \text{ GPa}, \quad (22)$$

$$\begin{aligned} &h_{111} = -1350 \text{ GPa}, \quad h_{112} = -800 \text{ GPa}, \\ &h_{123} = -120 \text{ GPa}, \quad h_{144} = -66 \text{ GPa}, \\ &h_{155} = -720 \text{ GPa}, \quad h_{456} = -32 \text{ GPa}. \end{aligned} \quad (23)$$

The values of the third order will be needed in the next Section. Taking into account the values (22) we obtain the following coefficients

Table 2
The components of linear stress and inclination angle ξ for copper

	t_{n1} [GPa]	t_{t1} [GPa]	ξ [radian]
$n_i^{(1)}$	169.00	0	0
$n_i^{(2)}$	202.15	24.86	.122
$n_i^{(3)}$	220.80	0	0
$n_i^{(4)}$	230.39	10.85	.047
$n_i^{(5)}$	238.07	0	0
$n_i^{(6)}$	201.54	29.06	.143
$n_i^{(7)}$	220.80	20.55	.093
$n_i^{(8)}$	232.09	15.21	.065

Note that for the directions $n_i^{(1)}$, $n_i^{(3)}$ and $n_i^{(5)}$ the stress is purely normal to the surface. The real stresses may be obtained by multiplication of the values in columns t_{n1} and t_{t1} by ν. The inclination angles are different from those quoted in the Table 1.

3. Nonlinear terms

There exist two kinds of the nonlinearity of the stress-strain relation. First of them is the physical nonlinearity. It manifests itself in the presence of the elastic constants of the third order. For the cubic symmetry there exist six different elastic constants of the third order. In the abbreviated notation these constants are h_{111}, h_{112}, h_{123}, h_{144}, h_{155} and h_{456}. In the tensor notation the non-zero elastic constants are c_{111111}, c_{111122}, c_{112233}, c_{112323}, c_{113131}, c_{233112}. Other non-zero components follow from the tensor symmetries. The elastic constants of second order contribute to stress proportional to ν^2.

The second kind of nonlinearity is of another origin. Because in the expression for deformation ε_{ij} the nonlinear product $u_{r,i}u_{r,j}$ is present, even in physically linear material the nonlinear terms occur. This fact is the source of geometrical nonlinearity. It manifests itself in the non-zero values of s_{n2}, s_{t2}.

We start with the geometrical nonlinearity. For $h_{11} = 1$, $h_{12} = 1$ and $h_{44} = 1$ and the eight directions $(\vartheta, \varphi)^{(K)}$ selected in the previous Section the values of longitudinal and transverse forces are given in the Table 3. In order to obtain stress in any material the values given in the Table must be multiplied by ν^2 and the value of elastic constant of the second order for that particular material. The values 1.571 marked by an asterisk were calculated as the limiting values.

Table 3
Coefficients t_{n2}, t_{t2} and ξ for the geometrical nonlinearity

	$h_{11}=1$			$h_{22}=1$			$h_{44}=1$		
	t_{n2}	t_{t2}	ξ	t_{n2}	t_{t2}	ξ	t_{n2}	t_{t2}	ξ
$n_i^{(1)}$	1.500	0	0	0	0	1.571*	0	0	1.571*
$n_i^{(2)}$	1.020	.120	.117	.480	.120	.245	.960	.240	.245
$n_i^{(3)}$	.750	0	0	.750	0	0	1.500	0	0
$n_i^{(4)}$	.611	.052	.086	.889	.052	.059	1.778	.105	.059
$n_i^{(5)}$	.500	0	0	1.000	0	0	2.000	0	0
$n_i^{(6)}$	1.029	.140	.135	.471	.140	.289	.942	.281	.289
$n_i^{(7)}$	.750	.099	.131	.750	.099	.131	1.500	.198	.131
$n_i^{(6)}$	.585	.073	.125	.913	.073	.080	1.827	.147	.080

Note that for the directions $n_i^{(1)}$, $n_i^{(3)}$ and $n_i^{(5)}$ the second order geometrical nonlinearity stress is purely normal to the surface.

For copper the coefficients for geometrical nonlinearity are given in Table 4. The inclination angles are rather small, do not exceed 0.05 radians.

Table 4
Geometrical nonlinearity for copper

	t_{n2} [GPa]	t_{t2} [GPa]	ξ [radian]
$n_i^{(1)}$	253.50	0	0
$n_i^{(2)}$	303.23	12.43	.041
$n_i^{(3)}$	331.20	0	0
$n_i^{(4)}$	345.59	5.43	.016
$n_i^{(5)}$	357.10	0	0
$n_i^{(6)}$	302.30	14.53	.048
$n_i^{(7)}$	331.20	10.28	.031
$n_i^{(8)}$	348.14	7.60	.022

Pass to the physical nonlinearity. Tables 5 and 6 give the longitudinal and transverse stress separately for each elastic constant of the third order.

Table 5
Coefficients t_{n3}, t_{t3} and ξ for $h_{111} = 1$, $h_{112} = 1$, $h_{123} = 1$

	$h_{111} = 1$			$h_{112} = 1$			$h_{123} = 1$		
	t_{n3}	t_{t3}	ξ	t_{n3}	t_{t3}	ξ	t_{n3}	t_{t3}	ξ
$n_i^{(1)}$	.500	0	0	0	0	1.571*	0	0	1.571*
$n_i^{(2)}$	.260	.120	.432	.240	.120	.464	0	0	1.571*
$n_i^{(3)}$	.125	0	0	.375	0	0	0	0	1.571*
$n_i^{(4)}$	.088	.029	.318	.346	.017	.050	.066	.047	.615
$n_i^{(5)}$	.056	0	0	.333	0	0	.111	0	0
$n_i^{(6)}$	.275	.128	.435	.205	.102	.461	.020	.026	.899
$n_i^{(7)}$	.145	.084	.524	.316	.062	.195	.039	.042	.813
$n_i^{(8)}$	.087	.056	.572	.325	.022	.066	.088	.045	.374

Table 6
Coefficients t_{n3}, t_{t3} and ξ for $h_{144} = 1$, $h_{155} = 1$, $h_{456} = 1$

	$h_{144} = 1$			$h_{155} = 1$			$h_{456} = 1$		
	t_{n3}	t_{t3}	ξ	t_{n3}	t_{t3}	ξ	t_{n3}	t_{t3}	ξ
$n_i^{(1)}$	0	0	1.571*	0	0	1.571*	0	0	1.571*
$n_i^{(2)}$	0	0	1.571*	.960	.480	.464	0	0	1.571*
$n_i^{(3)}$	0		1.571*	1.500	0	0	0	0	1.571*
$n_i^{(4)}$	.395	.279	.615	1.383	.070	.050	.527	.372	.615
$n_i^{(5)}$	.667	0	0	1.333	0	0	.889	0	0
$n_i^{(6)}$	.122	.153	.899	.820	.408	.461	.162	.204	.899
$n_i^{(7)}$	.236	.250	.813	1.264	.250	.195	.315	.333	.813
$n_i^{(8)}$	.528	.207	.374	1.299	.086	.066	.703	.276	.374

The values given in Tables 5 and 6 represent the physical nonlinearity. In order to obtain stresses for a definite material the coefficients t_{n3}, t_{t3} quoted in Tables 6 and 7 must be multiplied by ν^2 and additionally by the value of elastic constant of the third order for that particular material. The values 1.571 marked by asterisk were calculated as the limiting values. The inclination angle for physical nonlinearity is much larger than that for geometrical nonlinearity. For directions where stresses are small it reaches 90^{circ}. Obviously again for the directions $n_i^{(1)}$, $n_i^{(3)}$ and $n_i^{(5)}$ the stress is purely normal to the surface.

Table 7

Physical nonlinearity for copper

	t_{n3} [GPa]	t_{t3} [GPa]	ξ [radian]
$n_i^{(1)}$	−675.00	0	0
$n_i^{(2)}$	−1234.20	279.60	.223
$n_i^{(3)}$	−1548.75	0	0
$n_i^{(4)}$	−1442.37	67.59	.047
$n_i^{(5)}$	−1387.44	0	0
$n_i^{(6)}$	−1141.18	222.93	.193
$n_i^{(7)}$	−1388.44	140.99	.101
$n_i^{(8)}$	−1381.08	30.33	0.022

Note that for extension the longitudinal stresses t_{n3} are negative in contrast to the longitudinal stresses t_{n2} quoted in the Table 4, that are positive.

Finally consider jointly both physical and geometrical nonlinearities for copper. Table 8 gives the corresponding values, again for the eight directions selected above.

Table 8
Geometrical and physical nonlinearity for copper

	$t_{n2} + t_{n3}$ [GPa]	$t_{t2} + t_{t3}$ [GPa]	ξ [radian]
$n_i^{(1)}$	−421.50	0	0
$n_i^{(2)}$	−930.97	267.17	.279
$n_i^{(3)}$	−1217.55	0	0
$n_i^{(4)}$	−1096.79	73.02	.066
$n_i^{(5)}$	−1030.34	0	0
$n_i^{(6)}$	−838.87	208.39	.243
$n_i^{(7)}$	−1057.24	134.18	.126
$n_i^{(8)}$	−1032.95	22.73	.022

For elongation in the symmetry directions $n_i^{(1)}$, $n_i^{(3)}$ and $n_i^{(5)}$ shear stress $t_{t2}+t_{t3}$ and angle ξ are equal to zero. The geometrical and physical nonlinearities neutralize to some extent each other. Therefore the actual inclination angles for copper are in general smaller than those quoted separately in the Tables 4 and 7.

4. Extreme values

In the present Section the extreme values will be analyzed. The shearing planes and shearing directions for which one of coefficients s_{n1}, s_{n2}, s_{t3}, … reaches its extremum will be found. Their sums e.g. $s_{n2}+s_{n3}$, will be considered, too. The three components of the vector n_i are the independent variables. Three constraints expressing the fact, that n_{i1} is a unit vector must be taken into account. In order to avoid these constraints in the computations introduce two new, real parameters (ϑ,φ). Write the components of the vector n_i in the form

$$n_1 = \sin\vartheta\cos\varphi, \tag{24}$$

$$n_2 = \sin\vartheta\sin\varphi, \tag{25}$$

$$n_3 = \cos\vartheta. \tag{26}$$

Since n_i is the unit vector two parameters (ϑ,φ) define it uniquely. They may be interpreted as two angles. The angle ϑ defines the inclination of the unit vector n_i to the x_3 axis. The angle φ defines the inclination of its projection on the x_1x_2 plane to the x_1 axis. Note that the reflections of n_i in the coordinate planes are described by the following changes of the angles ϑ and φ

$$\begin{aligned}
(n_1,n_2,n_3) &\Rightarrow (-n_1,n_2,n_3) \text{ if } (\vartheta,\varphi) \Rightarrow (\vartheta,\pi-\varphi),\\
(n_1,n_2,n_3) &\Rightarrow (n_1,-n_2,n_3) \text{ if } (\vartheta,\varphi) \Rightarrow (\vartheta,-\varphi),\\
(n_1,n_2,n_3) &\Rightarrow (n_1,n_2,-n_3) \text{ if } (\vartheta,\varphi) \Rightarrow (\vartheta,\pi-\varphi).
\end{aligned} \tag{27}$$

Substitution of (24)–(26) into the expression for t_1 given in (16) leads to a sum of 81 products of trigonometric functions of ϑ and φ. Some terms due to symmetry of the problem are equal to zero. The same number of products appears in the expressions for t_2 and t_3 given in (17) and (18). Purely analytical approach to the extreme values leads to simple, but long trigonometric equations. In practice only the numerical approach is effective.

In cubic crystals all three principal directions are equivalent. Therefore the properties for some deformations are exactly the same, as the properties for other deformations. It is easy to check that the following changes of the deformation direction

$$\begin{aligned}
(n_1,n_2,n_3) &\Rightarrow (n_2,n_1,n_3),\\
(n_1,n_2,n_3) &\Rightarrow (n_1,n_3,n_2),\\
(n_1,n_2,n_3) &\Rightarrow (n_3,n_2,n_1)
\end{aligned}$$

do not change the properties of the crystal, i.e. the values of t_k. The above discussed symmetry properties of functions t_k allow us to confine all calculations to directions defined by the vector n_i possessing non-negative components n_1, n_2 and n_3. The values for other vectors n_i follow from the symmetries of the considered problem.

Start with the values of s_{k1}, s_{n1}, s_{b1}. They express the linear part of the stress-deformation function for pure shear.

Table 9
Extreme values of s_{n1}, s_{t1} and ξ for Cu

		Value	(ϑ,φ)	(n_1,n_2,n_3)
t_{n1}	max	238.1	(.9541,.7854)	(.577,.577.577)
	m/m	220.8	(.7854,0)	(.707,0,.707)
	min	169.0	$(0,\varphi)$	(0,0,1)
t_{t1}	max	29.1	(.4454,.7854)	(.305,.305,.902)
	m/m	25.9	(.3927,0)	(.383,0,.924)
	m/m	10.9	(.8368,.4460)	(.670,.320,.670)
	min	0	$(0,\varphi)$	(0,0,1)
	min	0	(.7854,0)	(.707,0,.707)
	min	0	(.9541,.7854)	(.577,.577.577)
ξ	max	.145	(.3933,.7854)	(.271,.271,.924)

Maximum value is marked by "max", and minimum value by "min". An extremum, that is neither maximum, nor minimum is marked by "m/m" (minimax). The values of ϑ, φ are useful only in computations. For analysis of the problem more useful and transparent is the direction (n_1,n_2,n_3) given in the last column. Note that in accord with (19) the components (n_1,n_2,n_3) may be interchanged, i.e. to (n_1,n_3,n_2). For $\alpha=\pi/2$ the normal to the shearing plane and the shearing direction coincide with the coordiate axes. If instead of a numerical value of φ is written φ then for each φ is reached an extremum.

The transverse force has a minimum for all symmetry directions (0,0,1), (1,0,1) and (1,1,1) three (and the 23 other equivalent symmetry directions). For these directions stress vector is parallel to n_i and the inclination angle has a minimum equal to 0. There exist no other minima of ξ. In order to save space the minima of ξ were not quoted.

Similar calculations lead to the extreme values of t_{n2}, t_{t2}. Their values are given in Table 10. Note that some of the directions in Table 5 and Table 6 do not coincide. The extreme direction for the geometrical nonlinearity are different from that for the physical nonlinearity.

Table 10
Extreme values of s_{n2}, s_{t2} and ξ for Cu

		Value	(ϑ,φ)	(n_1,n_2,n_3)
t_{n2}	min	357.1	(.9552,.7854)	(.577,.577,.577)
	max	331.2	(.7854,0)	(.707,0,.707)
	m/m	253.5	$(0,\varphi)$	(0,0,1)
t_{t2}	max	14.5	(.4449,.7854)	(.303,.303,.903)
	m/m	12.9	(.3924,0)	(.382,0,.924)
	m/m	5.43	(.8335,.4319)	(.673,.309,.673)
	min	0	$(0,\varphi)$	(0,0,1)
	min	0	(.7854,0)	(.707,0,.707)
	min	0	(.9552,.7854)	(.577,.577,.577)
ξ	max	.278	(.2918,0)	(.288,0,.958)
	.049	(.3931,.7854)	(.271,.271,.924)	

The physical nonlinearity is characterized by the data quoted in Table 11.

Table 11
Extreme values of s_{n3}, s_{t3} and ξ for Cu

		Value	(ϑ,φ)	(n_1,n_2,n_3)
t_{n3}	max	−1548.7	(.784,0)	(.707,0,.707)
	m/m	−1387.5	(.9553,.7854)	(.577,.577,.577)
	min	−.675	$(0,\varphi)$	(0,0,1)
t_{t3}	max	291.2	(.3931,0)	(.383,0,.924)
	m/m	245.8	(.3390,.7854)	(.235,.235,.943)
	m/m	73.5	(.8203,.3695)	(.682,.263,.682)
	min	0	$(0,\varphi)$	(0,0,1)
	min	0	(.784,0)	(.707,0,.707)
	min	0	(.9553,.7854)	(.577,.577,.577)
ξ	max	.278	(.2918,0)	(.288,0,.958)

All explanations given for Table 10 remain valid.

Since both s_{k2} and s_{k3} contribute to the stress proportionally to ν^2, important for the analysis is their sum $(s_{k2}+s_{k3})$. The same holds for the sums $(s_{n2}+s_{n3})$ and $(s_{b2}+s_{b3})$. Table 12 gives the corresponding extremes.

Table 12
Extreme values of $(s_{n2}+s_{n3})$, $(s_{t2}+s_{t3})$ and ξ for Cu

		Value	(ϑ,φ)	(n_1,n_2,n_3)
$t_{n2}+t_{n3}$	max	−421	$(0,\varphi)$	(0,0,1)
$t_{n2}+t_{n3}$	m/m	−1030, 3	(.9541,.7854)	(.577,.577,.577)
$t_{n2}+t_{n3}$	min	−1217.5	(.7854,0)	(.707,0,.707)
$t_{t2}+t_{t3}$	max	206.21	(.4456,.7854)	(.305,.305,.902)
$t_{t2}+t_{t3}$	max	278.3	(.3938,0)	(.384,0,.924)
$t_{t2}+t_{t3}$	M/m	232.3	(.3349,.7854)	(.233,.233,.944)
$t_{t2}+t_{t3}$	min	0	(.9541,.7854)	(.577,.577,.577)
η	max	.370	(.2730,0)	(.270,0,.963)
η	m/m	.280	(.3930,.8022)	(.266,.275,.924)
η	m/m	.346	(.2434,.7854)	(.171,.171,.971)
η	m/m	.070	(.8246,.3909)	(.679,.279,.679)
η	min	0	(.7854,0)	(.707,0,.707)

The three directions (1,0,0), (1,1,0) and (1,1,1) are connected with the symmetry of the cube. To them correspond extreme values of all three variables quoted in the Tables 9–12. Other directions, e.g. the direction (.305,.305,.902) in Table 12 is an extreme direction for one variable only. Such directions are specific extreme directions of the considered material.

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