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Pure shear of a cubic crystal

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Large simple shear 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 for three shearing planes and three directions for each plane has been calculated. The stresses have been calculated separately for each material constant. For copper, the shearing planes and shearing directions for which stress reaches extreme values have been determined. The extreme values for each component of the traction have been calculated.

1. Introduction

Crystals are of special interest in fundamental research. 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 possess the highest symmetry. Their mechanical behavior in the linear case is described by three elastic constants. Triclinic crystals belong to the class of the lowest symmetry. In the linear case they are described by twenty-one elastic constants.

Isotropic materials possess higher symmetry. Mechanical properties of linear isotropic material may be described by two elastic constants only. Isotropic crystals do not exist. Typical isotropic material is an amorphous material, e.g. glass. Approximation of an isotropic material is a polycrystalline cluster of randomly oriented crystals. Most of the experience in engineering is connected with isotropic materials. Manufactured pieces of single crystals are frequently used in physical experiments and physical equipment.

External load applied to a crystal results in a deformation. Since a crystal is not isotropic, its stress field differs from that of an isotropic material. The present paper aims at analysis of the forces, necessary to result in a shearing given in advance.

All 32 symmetry groups may be analyzed for linear and for the nonlinear material. Obviously a linear material, due to simplicity, is of special interest. Nonlinearity is manifested in the additional phenomena. Trying to avoid complex, non-transparent considerations, we do not consider general elasticity, but confine ourselves 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 are based on [1]. We confine the analysis to one symmetry only, namely to the cubic symmetry. Typical material of this symmetry is the crystal of copper.

Common for all theories is the notion of the strain tensor. 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 displacement vector u_i is a function of the Cartesian coordinates x_j and time $t, u_i = u_i\ (x_j, t)$. In the whole paper we compare two states only and time serves only as a 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, [1]

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,i} + u_{j,i} + u_{r,i}\, u_{r,j}\right). \tag{1.1}$$

The nonlinear product $u_{r,i}\, u_{r,j}$ is present in this expression. Therefore the deformation tensor ε_{ij} is always a nonlinear function of the displacement gradient. The linear measure of strain disregarding this term may be used only in the linear theory, where the stress is a linear function of strain.

The relation (1.1) is purely geometrical. No material properties are involved. The elastic energy (strain energy) is a nonlinear function of strain ε_{ij}. Second order elasticity is the simplest generalization of the linear elasticity. The expression for the elastic energy Φ (per unit volume in the stress-free state) takes into account the cubes, but neglects the fourth higher powers of strain tensor ε_{ij}. The elastic energy Φ reads

$$\Phi = \frac{1}{2}\, c_{ijkm}\, \varepsilon_{ij}\, \varepsilon_{km} + \frac{1}{6}\, c_{ijkmrs}\, \varepsilon_{ij}\, \varepsilon_{km}\, \varepsilon_{rs}. \tag{1.2}$$

It is a cubic function of strain, but polynomial of the sixth order in the displacement gradient. The coefficients 1/2 and 1/6 are commonly accepted in the literature, [2].

Summation convention is accepted in the whole present paper. The tensor c_{ijkm} is the tensor of second order elastic constants and c_{ijkmrs} is the tensor of third order elastic constants. In some older papers these tensors are called first and second order elastic constants, respectively. Since the expression (1.1) is homogeneous in ε_{ij} it may be assumed that $c_{ijkm} = c_{kmij}$ and $c_{ijkmrs} = c_{kmijrs} = c_{ijrskm}$. Since ε_{ij} is symmetric, it may be assumed without loosing the generality that the constants satisfy the relations $c_{ijkm} = c_{jikm}$ and $c_{ijkmrs} = c_{jikmrs}$.

The elastic constants of the second order and of the third order may be therefore assumed to posses the following symmetries

$$c_{ijkm} = c_{kmij} = c_{jikm}, \tag{1.3}$$

$$c_{ijkmrs} = c_{kmijrs} = c_{ijrskm} = c_{jirskm}. \tag{1.4}$$

Symmetry of the crystal results in additional symmetries. As mentioned above, the second order elastic constants c_{ijkm} for triclinic symmetry may be expressed by 21 independent material constants. In the simplest case of cubic symmetry there are only 3 non-zero independent constants of the second order and 6 material constants of the third order. The 81 constants c_{ijkm} and 729 constants c_{ijkmrs} may therefore for the cubic crystal be expressed by only 9 elastic constants. The isotropic material is characterized by only 5 elastic constants, namely 2 constants of second order (Lamé constants) and 3 constants of third order.

There exist at least eight different methods of measuring the constants of the third order. The 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}

$$H_{ij} = \frac{\partial \Phi}{\partial \varepsilon_{ij}} + \frac{\partial \Phi}{\partial \varepsilon_{ji}}. \tag{1.5}$$

From (1.2) and the symmetries (1.3)–(1.4) there follows

$$\frac{\partial \Phi}{\partial \varepsilon_{ij}} = c_{ijkm}\,\varepsilon_{km} + \frac{1}{2} c_{ijkmrs}\,\varepsilon_{km}\,\varepsilon_{rs}, \tag{1.6}$$

and further

$$H_{ij} = 2c_{ijkm}\varepsilon_{km} + c_{ijkmrs}\,\varepsilon_{km}\,\varepsilon_{rs}. \tag{1.7}$$

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

$$2\tau_{ij} = H_{ij} + H_{ir}u_{j,r}. \tag{1.8}$$

The stress tensor τ_{ij} is not symmetric. It is in fact the first Piola-Kirchhoff stress tensor. This tensor may be expressed by the deformation gradient and material constants. Full expression for τ_{ij} will be given further for simple shear.

The most important mechanism of deformation of a crystal is simple shear, [4]. This deformation induces relatively small change of the volume. Consider simple shear of a crystal of arbitrary symmetry. Denote by n_i the normal to the shearing plane and by k_i the shearing direction. Both vectors are unit vectors and orthogonal to each other

$$k_i k_i = 1, \quad n_i n_i = 1, \quad k_i n_i = 0. \tag{1.9}$$

In the case of shear in the direction k_i, the displacement vector u_i has the direction of k_i and is proportional to the distance $n_r x_r$ from the plane $n_r x_r$=0. The displacement u_i for hear reads

$$u_i(x_r) = \nu k_i n_r x_r, \tag{1.10}$$

where ν is the measure of shear. For the whole plane $n_r x_r$=const the displacement vector is the same. The strain tensor ε_{ij} may now be calculated from (1.1) and (1.10). For each material, linear and nonlinear, it consists of a term proportional to ν and a term proportional to ν^2

$$2\varepsilon_{ij} = \nu\left(k_i n_j + k_j n_i\right) + \nu^2 n_i n_j. \tag{1.11}$$

Substitute the above expression into (1.8) and take into account the symmetries of c_{ijkm} and c_{ijkmrs} to obtain the following expression for the stress tensor:

$$\tau_{ij} = \nu c_{ijpq} k_p n_q + \nu^2\left(\frac{1}{2} c_{ijpqrs} k_p k_r n_q n_s + \frac{1}{2} c_{ijpq} n_p n_q + c_{impq} k_j k_p n_m n_q\right). \tag{1.12}$$

The stress tensor is uniquely determined by the strain energy Φ and the shear. In (1.12) the terms of the order ν^3 have been neglected, since already Φ does not take into account the third powers of ε_{ij}. The stress vector t_i acting on a surface with unit normal n_i equals the product of the stress tensor τ_{ij} and the vector n_i

$$t_j = \nu c_{ijpq} k_p n_i n_q + \nu^2\left(\frac{1}{2} c_{ijpqrs} k_p k_r n_i n_q n_s + \frac{1}{2} c_{ijpq} n_i n_p n_q + k_j c_{impq} k_p n_i n_m n_q\right). \tag{1.13}$$

In general this vector is neither perpendicular, nor collinear with k_i or n_i. The component of t_j in the shear direction k_i equals $t_j k_j$. Define the vector b_i as the vector product of k_i and n_i

$$b_i = \varepsilon_{irs} k_r n_s, \tag{1.14}$$

where ε_{irs} is the permutation symbol. This unit vector is orthogonal to k_i and n_i.

Define three components s_k, s_n, s_b of the stress vector as the scalar products of the stress vector and the unit vectors k_i, n_i, and b_i

$$s_k = t_j k_j, \quad s_n = t_j n_j, \quad s_b = t_j b_j. \tag{1.15}$$

In accord with the above relations there hold the relations

$$\begin{aligned} s_k &= \nu s_{k1} + \nu^2 (s_{k2} + s_{k3}), \\ s_n &= \nu s_{n1} + \nu^2 (s_{n2} + s_{n3}), \\ s_b &= \nu s_{b1} + \nu^2 (s_{b2} + s_{b3}), \end{aligned} \tag{1.16}$$

where

$$\begin{aligned} s_{k1} &= c_{ijpq} k_i n_j k_p n_q, \\ s_{k2} &= \frac{3}{2} c_{ijpq} k_i n_j k_p n_q, \\ s_{k3} &= \frac{1}{2} c_{ijpqrs} k_i n_j k_p n_q k_r n_s. \end{aligned} \tag{1.17}$$

$$\begin{aligned} s_{n1} &= c_{ijpq} n_i n_j k_p n_q, \\ s_{n2} &= \frac{1}{2} c_{ijpq} n_i n_j n_p n_q, \\ s_{n3} &= \frac{1}{2} c_{ijpqrs} n_i n_j k_p n_q k_r n_s. \end{aligned} \tag{1.18}$$

$$\begin{aligned} s_{b1} &= c_{ijpq} b_i n_j k_p n_q, \\ s_{b2} &= \frac{3}{2} c_{ijpq} b_i n_j k_p n_q, \\ s_{b3} &= \frac{1}{2} c_{ijpqrs} b_i n_j k_p n_q k_r n_s. \end{aligned} \tag{1.19}$$

The projections of t_i on n_i and on b_i , i.e. the scalar products $t_i n_i$ and $t_i b_i$ in linear elasticity of isotropic material are equal to zero. In nonlinear elasticity the projection of t_i on n_i is different from zero, even for isotropic material. In fact this stress component for isotropic material is always negative. For anisotropic material both projections are in general different from zero. The parameter s_k

introduced above is a measure of the projection of the stress vector on the direction k_i.

Each of the expressions for s_k, s_n, s_b consists of a part proportional to the amount of shear ν and a part proportional to the squared amount of shear ν^2. The parts s_{k1}, s_{n1}, s_{b1} do not take into account the nonlinearity and are exactly the same as in linear elasticity. The other parts take into account nonlinearity. More exactly, the other parts express the second term of the Taylor expansion of stress vector t_i. For infinitesimal shear ν the first terms s_{k1}, s_{n1}, s_{b1} in (1.17)–(1.19) are the leading terms. For other ν the second and third terms must be taken into account. In the next chapter we analyze separately the terms of (1.16)–(1.18).

Shear stiffness s equals the ratio of the component of t_j in the shear direction k_j and the measure of shear ν. Stiffness is equal to the sum

$$s = s_{k1} + \nu(s_{k2} + s_{k3}). \tag{1.20}$$

2. Linear elasticity

Analysis of the present chapter is based on the principal terms of s_{k1}, s_{n1}, s_{b1}, namely on the relations

$$\begin{aligned} s_{k1} &= c_{ijpq} k_i n_j k_p n_q, \\ s_{n1} &= c_{ijpq} n_i n_j k_p n_q, \\ s_{b1} &= c_{ijpq} b_i n_j k_p n_q. \end{aligned} \tag{2.1}$$

Since b_i as the vector product of n_i and k_i may be expressed by n_i and k_i, the above functions depend on n_i and k_i only. Note that s_{k1} is an even function of n_i and k_i; s_{n1} is an odd function of n_i and an odd function of k_i; finally s_{b1} is an odd function of n_i and even function of k_i.

In the present paper we consider only one definite material symmetry, namely the cubic symmetry. Other crystal symmetries may be treated in the same way. In the linear theory there exist only three independent elastic constants of cubic crystal. In 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 tensor c_{ijpq} may be expressed by the three constants h_{11}, h_{12} and h_{44}, namely

$$\begin{aligned} &c_{1111} = c_{2222} = c_{3333} = h_{11}, \\ &c_{1122} = c_{1133} = c_{2233} = c_{2211} = c_{3311} = c_{3322} = h_{12}, \\ &c_{2323} = c_{2332} = c_{3223} = \ldots = c_{1212} = c_{1221} = h_{44}. \end{aligned} \tag{2.2}$$

The remaining components of the tensor c_{ijpq} (elastic constants of the second order), e.g. the components c_{1231}, c_{1112}, are equal zero.

In order to gain better recognition of the stresses in this chapter we do not consider any specified real material, but aim to analyze the influence of elastic constants on stress in pure shear of cubic crystal. This fact suggests separate consideration of three cases: i) $h_{11} = 1,\ h_{12} = 0,\ h_{44} = 0$, ii) $h_{11} = 0, h_{12} = 1, h_{44} = 0$ and iii) $h_{11} = 0,\ h_{12} = 0,\ h_{44} = 1$.

Calculate the coefficients s_{k2}, s_{n2} and s_{b2} for three different shear planes (1,0,0), (1,1,0) and (1,1,1). For each shear plane three shearing planes were selected.

Consider first the shearing plane n_i=(1,0,0) and three different shearing directions

$$k_i^{(1)} = (0,1,0), \quad k_i^{(2)} = (0,1,1), \quad k_i^{(3)} = (0,1,1+\sqrt{2}). \tag{2.3}$$

The vector $k_i^{(3)} = (0,1,1+\sqrt{2})$ bisects the angle between the first two. Because of the symmetry of the problem, the values of s_{k2}, s_{n2} and s_{b2} for the directions $k_i^{(1)}$ and $k_i^{(2)}$ take extreme values.

The shearing plane n_i=(1,1,0) is equally inclined to the directions (1,0,0) and (0,1,0) and parallel to the direction (0,0,1). Three shearing directions

$$k_i^{(4)} = (1,-1,0), \quad k_i^{(5)} = (0,0,1), \quad k_i^{(6)} = (1,-1,\sqrt{2}) \tag{2.4}$$

are orthogonal to (1,1,0). The shearing directions $k_i^{(4)}$=(1,–1,0) and $k_i^{(5)}$ =(0,0,1) are the geometrical symmetry directions of the problem. The shearing direction $k_i^{(6)}$= (1,–1,$\sqrt{2}$) bisects the shearing directions $k_i^{(4)}$ and $k_i^{(5)}$.

The shearing plane n_i=(1,1,1) is equally inclined to the three directions (1,0,0), (0,1,0) and (0,0,1). The proposed shearing directions are

$$k_i^{(7)} = (2,-1,-1), \quad k_i^{(8)} = (1,-1,0), \quad k_i^{(9)} = (2+\sqrt{3},-1-\sqrt{3},-1). \tag{2.5}$$

The shearing directions $k_i^{(7)}$=(2,–1,–1) and $k_i^{(8)}$=(1,–1,0) are the symmetry directions of the problem. Direction (1,–2,1) is equivalent to the direction (2,–1,–1). Since (1,–1,0) bisects the directions (1,–2,1) and (2,–1,–1), it is a symmetry direction of the problem. The direction $k_i^{(9)}$ = (2+$\sqrt{3}$,–1–$\sqrt{3}$,–1) bisects the directions k_i =(1,–1,0) and k_i =(2,–1,–1).

The vectors $k_i^{(1)},\ k_i^{(2)}, ..., k_i^{(9)}$ and the corresponding shearing planes are listed in the first two columns of Table 1. In calculation, one of the elastic constants was assumed to be equal 1, the other two to be equal zero.The following values s_{k1}, s_{n1} and s_{b1} were calculated.

The values given in the first two columns are the components of the vector parallel to n_i and the vector parallel to k_i. In computations they must be normalized to obtain the vectors n_i and k_i of unit length. For the shearing plane

Table 1. Coefficients s_{k1}, s_{n1}, s_{b1} for copper.

n_i	k_i	$h_{11}=1,\ h_{12}=0,\ h_{44}=0$			$h_{11}=0,\ h_{12}=1,\ h_{44}=0$			$h_{11}=0,\ h_{12}=0,\ h_{44}=1$		
		s_{k1}	s_{n1}	s_{b1}	s_{k1}	s_{n1}	S_{b1}	s_{k1}	s_{n1}	s_{b1}
(1,0,0)	$k_i^{(1)}$	0	0	0	0	0	0	1	0	0
	$k_i^{(2)}$	0	0	0	0	0	0	1	0	0
	$k_i^{(3)}$	0	0	0	0	0	0	1	0	0
(1,1,0)	$k_i^{(4)}$	.500	0	0	–.500	0	0	0	0	0
	$k_i^{(5)}$	0	0	0	0	0	0	0	0	0
	$k_i^{(6)}$	.250	0	–.250	–.250	0	.250	.500	0	.500
(1,1,1)	$k_i^{(7)}$	.333	0	0	–.333	0	0	.333	0	0
	$k_i^{(8)}$	.333	0	0	–.333	0	0	.333	0	0
	$k_i^{(9)}$	.333	0	0	–.333	0	0	.333	0	0

Table 2. Coefficients s_{n2} for n_i=(1,0,0), n_i=(1,1,0) and n_i=(1,1,1).

n_i	k_i	$h_{11}=1$			$h_{12}=1$			$h_{44}=1$		
		s_{k2}	s_{n2}	s_{b2}	s_{k2}	s_{n2}	s_{b2}	s_{k2}	s_{n2}	s_{b2}
(1,0,0)	$k_i^{(1)}$	0	.500	0	0	0	0	1.500	0	0
	$k_i^{(2)}$	0	.500	0	0	0	0	1.500	0	0
	$k_i^{(3)}$	0	.500	0	0	0	0	1.500	0	0
(1,1,0)	$k_i^{(4)}$	.750	.250	0	–.750	.250	0	0	.500	0
	$k_i^{(5)}$	0	.250	0	0	.250	0	1.500	.500	0
	$k_i^{(6)}$	.375	.250	–.125	–.375	.250	.125	.750	.500	.250
(1,1,1)	$k_i^{(7)}$	.500	.167	0	–.500	.333	0	.500	.667	0
	$k_i^{(8)}$	.500	.167	0	–.500	.333	0	.500	.667	0
	$k_i^{(9)}$	.500	.167	0	–.500	.333	0	.500	.667	0

n_i=(1,0,0) and shearing directions k_i=(0,1,0), or k_i=(0,0,1), or k_i=(0,1,1), the values of s_{n1}, s_{k1}, s_{b1} are extreme values. Similarly, values for shearing plane n_i=(1,1,0) and shearing directions k_i=(1,–1,0), or k_i=(0,0,1), the values of s_{n1}, s_{k1}, s_{b1} are extreme values. For n_i=(1,1,1) there exist six equivalent shearing directions, one of them is k_i=(2,–1,–1). Next to it is situated the direction k_i=(1,–2,1). The vector k_i=(1,–1,0) bisects them. There exist six shearing directions equivalent to k_i=(1,–1,0). Because of the symmetry, the values of s_{k1}, s_{n1}, s_{b1} for n_i=(1,1,1), k_i=(2,–1,–1) or k_i=(1,–1,0) are extreme values. Table 2 gives the extreme values for copper.

3. Second order terms

For the cubic symmetry there exist six different elastic constants of the third order. In the abbreviated notation they 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 are the result of the tensor symmetries. The elastic constants of second order contribute stress of the order ν^2. Here we calculate the stresses for the same n_i and k_i as above.

The geometrical nonlinearity is manifested in the non-zero values of s_{k2}, s_{n2} and s_{b2}. For h_{11}=1, h_{12}=1 and h_{44}=1 they are given in the Table 2.

The values of s_{k3} , s_{n3} and s_{b3} represent the material nonlinearity. For h_{111}=1, h_{112}=1 and h_{123}=1 they are given in the Table 3.

Table 4 has exactly the same structure as Table 3. It gives the values of s_{k3}, s_{n3} and s_{b3} for h_{144}=1, h_{155} =1 and h_{456} =1.

Note that the shearing plane n_i and the shearing direction k_i may be arbitrarily chosen. The vector b_i is then uniquely defined as the vector product of n_i and k_i. According to (1.16)–(1.18), the function s_{k3} is an odd function of k_i and an odd function of n_i. In contrast s_{n3} is even function of k_i and even function of n_i. And finally s_{b3} is an odd function of b_i, even function of k_i and odd function of n_i. Since b_i as the vector product is an odd function of k_i and an odd function of n_i, the function s_{b3} is an odd function of k_i, and an even function of n_i. For fixed shearing plane, a change of the shearing direction k_i into the opposite direction

$$(k_1, k_2, k_3) \quad \Rightarrow (-k_1, -k_2, -k_3) \tag{3.1}$$

changes the signs of coefficients s_{k3} and s_{b3}, and does not change the value of s_{n3}.

With the cubic symmetry a physically more interesting, following invariance is connected. Simultaneous reflections of the vectors n_i and k_i in the (2.3), (3.1) and (1.2) coordinate planes

Table 3. Coefficients s_{k3}, s_{n3}, s_{b3} for $h_{111}=1$, $h_{112}=1$, $h_{123}=1$.

n_i	k_i	$h_{111}=1$, other $h_{\alpha\beta\gamma}=0$			$h_{112}=1$, other $h_{\alpha\beta\gamma}=0$			$h_{123}=1$, other $h_{\alpha\beta\gamma}=0$		
		s_{k3}	s_{n3}	s_{b3}	s_{k3}	s_{n3}	s_{b3}	s_{k3}	s_{n3}	s_{b3}
(1,0,0)	$k_i^{(1)}$	0	0	0	0	0	0	0	0	0
	$k_i^{(2)}$	0	0	0	0	0	0	0	0	0
	$k_i^{(3)}$	0	0	0	0	0	0	0	0	0
(1,1,0)	$k_i^{(4)}$	0	.125	0	0	–.125	0	0	0	0
	$k_i^{(5)}$	0	0	0	0	0	0	0	0	0
	$k_i^{(6)}$	0	.062	0	0	–.062	0	0	0	0
(1,1,1)	$k_i^{(7)}$	.039	.056	0	–.118	0	0	.079	–.056	0
	$k_i^{(8)}$	0	.056	–.039	0	0	.118	0	–.056	–.079
	$k_i^{(9)}$	.028	.056	–.028	–.083	0	.083	.056	–.056	–.056

Table 4. Coefficients s_{k3}, s_{n3}, s_{b3} for h_{144}=1, h_{155}=1, h_{456}=1.

n_i	k_i	h_{144}=1, other $h_{\alpha\beta\gamma}$=0			h_{155}=1, other $h_{\alpha\beta\gamma}$=0			h_{456}=1, other $h_{\alpha\beta\gamma}$=0		
		s_{k3}	s_{n3}	s_{b3}	s_{k3}	s_{n3}	S_{b3}	s_{k3}	s_{n3}	s_{b3}
(1,0,0)	$k_i^{(1)}$	0	0	0	0	1.000	0	0	0	0
	$k_i^{(2)}$	0	0	0	0	1.000	0	0	0	0
	$k_i^{(3)}$	0	0	0	0	1.000	0	0	0	0
(1,1,0)	$k_i^{(4)}$	0	0	0	0	0	0	0	0	0
	$k_i^{(5)}$	0	.500	0	0	.500	0	0	1.000	0
	$k_i^{(6)}$	0	.250	0	0	.250	0	0	.500	0
(1,1,1)	$k_i^{(7)}$	.236	–.333	0	–.236	.667	0	–.157	–.222	0
	$k_i^{(8)}$	0	–.333	–.236	0	.667	.236	0	–.222	.157
	$k_i^{(9)}$	.167	–.333	–.167	–.167	.667	.167	–.111	–.222	.111

$$(3.2)\qquad \begin{aligned} &(n_1,n_2,n_3) \Rightarrow (-n_1,n_2,n_3) \quad \text{and} \quad (k_1,k_2,k_3) \Rightarrow (-k_1,k_2,k_3),\\ &(n_1,n_2,n_3) \Rightarrow (n_1,-n_2,n_3) \quad \text{and} \quad (k_1,k_2,k_3) \Rightarrow (k_1,-k_2,k_3),\\ &(n_1,n_2,n_3) \Rightarrow (n_1,n_2,-n_3) \quad \text{and} \quad (k_1,k_2,k_3) \Rightarrow (k_1,k_2,-k_3). \end{aligned}$$

do not change s_{k3} and s_{n3}, and change the sign of s_{b3}. The proof based on the definitions of s_{k3}, s_{n3} and s_{b3} is elementary, but demands long calculations. It is easy to check the invariance (2.7) numerically.

4. Extreme values

In the present chapter will be analyzed the shearing planes and shearing directions for which the tractions reach extreme values. The coefficients s_{k1}, s_{n1}, s_{b1},, s_{k2}, ..., s_{b3} and their sums, e.g. $s_{k2}+ s_{k3}$, will be considered separately. The independent variables are the two vectors n_i and k_i. Three constraints expressing the fact that they are unit, mutually orthogonal vectors must be taken into account. In order to avoid the constraints in computations introduce three new, real parameters $(\vartheta, \varphi, \psi)$, which enable us to write the components of the unit vectors n_i and k_i in the form

$$(4.1)\qquad \begin{aligned} n_1 &= \sin\vartheta\, \cos\varphi,\\ n_2 &= \sin\vartheta\, \sin\varphi,\\ n_3 &= \cos\vartheta; \end{aligned}$$

$$(4.2)\qquad \begin{aligned} k_1 &= \cos\psi\, \cos\vartheta\, \cos\varphi - \sin\psi\, \sin\varphi,\\ k_2 &= \cos\psi\, \cos\vartheta\, \sin\varphi + \sin\psi\, \cos\varphi,\\ k_3 &= -\cos\psi\, \sin y\vartheta. \end{aligned}$$

The two angles ϑ and φ define the vector n_i, namely its inclination to the x_3 axis and inclination of its projection on the $x_1\, x_2$ plane to the x_1 axis. These two angles define the shearing plane. The additional angle ψ, together with ϑ and φ define the shearing direction k_i, which is parallel to the shearing plane. The vector b_i is uniquely defined by the vectors n_i and k_i, as their vector product

$$(4.3)\qquad \begin{aligned} b_1 &= -\sin\psi \cos\vartheta \cos\varphi - \cos\psi \sin\varphi,\\ b_2 &= -\sin\psi \cos\vartheta \sin\varphi + \cos\psi \cos\varphi,\\ b_3 &= \sin\psi \sin\vartheta. \end{aligned}$$

The triad of three mutually orthogonal unit vectors (n_i, k_i, b_i) possesses three degrees of freedom. It is uniquely defined by the three parameters ϑ, φ, ψ. For arbitrary (ϑ, φ, ψ) the above three unit vectors n_i, k_i and b_i are mutually orthogonal. The functions s_k, s_n, s_b depend on n_i, k_i and b_i. If it is taken into account that b_i may be expressed by n_i and k_i, then the functions s_k, s_n, s_b depend on n_i and k_i only.

Very useful for the description of material properties is the shearing plane defined by n_i and the shearing direction k_i. From (4.1) it follows that replacement of (ϑ, φ, ψ) by other values results in reflection in the shearing planes and shearing directions in the coordinate planes

$$
\begin{aligned}
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (-n_1, n_2, n_3),\ (-k_1, k_2, k_3) \\
&\qquad\qquad \text{if} \quad (\vartheta, \varphi, \psi) \quad \Rightarrow (\vartheta, \pi - \varphi, -\psi), \\
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (n_1, -n_2, n_3),\ (k_1, -k_2, k_3) \\
&\qquad\qquad \text{if} \quad (\vartheta, \varphi, \psi) \quad \Rightarrow (\vartheta, -\varphi, -\psi), \\
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (n_1, n_2, -n_3),\ (k_1, k_2, -k_3) \\
&\qquad\qquad \text{if} \quad (\vartheta, \varphi, \psi) \quad \Rightarrow (\vartheta, \pi - \varphi, -\psi).
\end{aligned} \tag{4.4}
$$

Substitution of (4.1)–(4.3) into the expression for s_k given in (1.16) leads to a sum of 225 products of trigonometric functions of ϑ, φ and ψ. Due to symmetry some terms are equal zero. The same number of products appears in the expressions for s_{n3} and s_{b3} given in (1.17) and (1.18). Purely analytical approach leads to simple, but long expressions. Finding the roots would be very tedious. In practice only the numerical approach is effective.

Confine our attention to one definite material, namely to copper. Copper has the cubic symmetry of the type VIIb for which there exist only three different elastic constants of the first order h_{11}, h_{12}, h_{44} and six different elastic constants of the second order h_{111}, h_{112}, h_{123}, h_{144}, h_{155}, h_{456}, cf. [2, 3]. The elastic constants of the second and third order for copper are

$$
h_{11} = 169\,\text{GPa}, \quad h_{12} = 122\,\text{GPa}, \quad h_{44} = 73.5\,\text{GPa}, \tag{4.5}
$$

$$
\begin{aligned}
&h_{111} = -1350\,\text{GPa}, \quad h_{112} = -800\,\text{GPa}, \quad h_{123} = -120\,\text{GPa}, \\
&h_{144} = -66\,\text{GPa}, \quad h_{155} = -720\,\text{GPa}, \quad h_{456} = -32\,\text{GPa}.
\end{aligned} \tag{4.6}
$$

In cubic crystals all three principal directions are equivalent. It is easy to check that the following changes of the shearing plane (n_1, n_2, n_3) and shearing direction (k_1, k_2, k_3)

$$
\begin{aligned}
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (n_2, n_1, n_3),\ (k_2, k_1, k_3), \\
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (n_1, n_3, n_2),\ (k_1, k_3, k_2), \\
&(n_1, n_2, n_3),\ (k_1, k_2, k_3) \Rightarrow (n_3, n_2, n_1),\ (k_3, k_2, k_1),
\end{aligned}
$$

do not change the properties of the crystal, i.e. the values of s_{k1}, s_{n1}, s_{b1} s_{k1},..., s_{b3}.

The above discussed symmetry properties of functions s_k, s_n, s_b allow us to confine all calculations to shearing planes defined by the vector n_i possessing non-negative components n_1, n_2 and $n_3, n_i > 0$. Such shearing planes are the most natural planes. The values for other vectors n_i, k_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 5. Extreme values of s_{k1}, s_{n1}, s_{b1} for Cu.

		Value	ϑ, φ, ψ	n_i	k_i
s_{k1}	max	75.30	(.393,0,1.571)	(.383,0,.924)	(0,1,0)
	m/m	36.45	(.785,.785,0)	(.500,.500,.707)	(.500,.500,–.707)
	min	23.50	(1.571,.785,1.571)	(.707,.707,0)	(–.707,.707,0)
s_{n1}	max	29.06	(1.261,.326,2.306)	(.902,.305,.305)	(–.431,.631,.646)
	m/m	0		(1,0,0)	(–.500,–.707,.500)
	min	–29.06	(1.263,1.245,.841)	(.305,.902,.305)	(–.638,.431,–.638)
s_{b1}	max	25.90	(–.785,3.142,.785)	(.707,0,.707)	(–.500,–.707,.500)
	m/m	0*	(1.571,0, 1.571)	(1,0,0)	(0,1,0)
	min	–25.90	(1.571,.785,.785)	(.707,.707,0)	(–.500,.500,–.707)

Maximum value is marked by "max", and minimum value by "min". An extremum, that is neither maximum, nor minimum (saddle point) is marked by "m/m". The value 0 marked by asterisk is an extremum for each ψ. For $\psi = \pi/2$ the normal to the shearing plane and the shearing direction coincide with the coordiate axes.

Pass now to the values of s_{k2}, s_{n2}, s_{b2}. They express the geometrical non-linearity of the deformation. Their values are given in Table 6. The value 84.50 marked by asterisk is an extremum for each ψ.

Table 6. Extreme values of s_{k2}, s_{n2}, s_{b2} for Cu.

		Value	ϑ, φ, ψ	n_i	k_i
s_{k2}	max	112.95	(0,.785,0)	(0,0,1)	(.707.–.707,0)
	m/m	54.68	(.785,.785,0)	(.500,.500,.707)	(.500,.500,–.707)
	min	35.25	(.785,0,0)	(.707,0,.707)	(.707,0,–.707)
s_{n2}	max	119.03	(.955,.785,.732)	(.577,.577,.577)	(–.169,.776,–.607)
	m/m	110.40	(.785,0,0)	(.707,0,.707)	(.707,0,–.707)
	min	84.50*	(0,.785,0)	(0,0,1)	(.707,.707,0)
s_{b2}	max	38.85	(.785,1.571,.785)	(0,.707,.707)	(–.707,.500,–.500)
	min	–38.85	(1.571,.785,.785)	(.707,.707,0)	(–.500,.500,–.707)

Similar calculations lead to the extreme values of s_{k3}, s_{n3}, s_{b3}. Their values are given in Table 7. Note that some of the directions in Table 6 and Table 7 do not coincide. The extreme directions for the geometrical nonlinearity are different from that for the physical nonlinearity.

Table 7. Extreme values of s_{k3}, s_{n3}, s_{b3} for Cu.

		value	ϑ,φ,ψ	n_i	k_i
s_{k3}	max	160.59	(1.047,.615–.956)	(.707,.500,.500)	(.707.–.500,–.500)
	max	64.82	(.228,.785,0)	(.159,.159,.974)	(.689,.689,–.226
	min	–64.82	(–.228,3.927,0)	(.150,.150,.974)	(–.689,–.689,.226)
	min	–160.59	(.785,.785,0)	(.500,.500,.707)	(.500,.500,–.707
s_{n3}	max	–68.75	(.785,0,0)	(.707,0,.707)	(.707,0,–.707)
	max	–109.69	(.555,.785,0)	(.372,.372,.850)	(.601,.601,–.527
	min	–360.0	(0,.785,0)	(0,0,1)	(.707,.707,0)
	min	–395.15	(1.211,.385,.715)	(.868,.352,.352)	(0,.707,–.707)
S_{b3}	max	125.24	(.887,.952,.423)	(.450,.632,.632)	(0,.707,–.707)
	max	73.75	(–.393,3.142,1.571)	(.383,0,.924)	(0,–1,0)
	min	–73.75	(.393,0,1.571)	(.383,0,.924)	(0,1,0)
	min	–125.24	(1.104,.785,1.571)	(.632,.632,.450)	(–.707,.707,0)

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 8 gives the corresponding extreme values.

Table 8. Extreme values of $(s_{k2} + s_{k3})$, $(s_{n2}+ s_{n3})$, $(s_{b2} + s_{b3})$.

		value	$\vartheta,\varphi\ \ ,\psi$	n_i	k_i
$s_{k2}+s_{k3}$	max	215.27	(1.047,.615–.956)	(.707,.500,.500)	(.707.–.500,–.500)
	max	167.72	(.201,.785,0)	(.141,.141,.980)	(.693,.693,–.200
	min		(–.230,3.824,.125)	(.177,.144,.974)	(–.671,–.706,.226)
	min	35.45	(–.258,3.903,.026)	(.185,.176,.967)	(–.684,–.684,.255)
	min	–105.92	(.785,.785,0)	(.500,.500,.707)	(.500,.500,–.707
$s_{n2}+s_{n3}$	max	41.65	(.785,0,0)	(.707,0,.707)	(.707,0,–.707)
	max	–2.05	(.569,.785,0)	(.381,.381,.841)	(.596,.596,–.538
	max	–102.10	(1.571,.785,0)	(.707,.707,0)	(0,0,–1.000)
	min	–275.50	(0,.785,0)	(0,0,1)	(.707,.707,0)
	min	–291.9	(1.264,.323,.731)	(.904,.302,.302)	(0,.707,–.707)
$s_{b2}+s_{b3}$	max	126.35	(.861,.938,.462)	(.448,.611,.652)	(–.014,.734,–.679)
	max	75.79	(–.401,3.202,1.435)	(.024,.921,.389)	(–.996,.054,–.065)
	min	–53.2	(–.291,4.137,–.785)	(.156,.611,.448)	(–.962,–.184,.203)
	min	–75.79	(.401,1.512,1.704)	(.023,.390,.921)	(–.997,–.064,.052)
	min	–126.35	(1.060,.753,1.553)	(.652,.611,.448)	(.678,.735,–.016

The angles (ϑ,φ,ψ) make easier the computations. Obviously, instead of the angles (ϑ,φ,ψ) the two vectors n_i, k_i may be used. Since for cubic symmetry all three directions in space are equivalent, some shearings are physically equivalent.

Note that some directions in the above tables coincide e.g. the direction (.500,.500,.707) is a common extreme direction for s_{k2} and s_{k3} (Tables 6 and 7). Such directions are in fact connected with the symmetry of the problem. Other directions, e.g. (.652,.611,.448) in the last line of Table 8 is an extreme direction for one set of elastic constants only. Such directions are specific extreme directions for one material only, namely copper.

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