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 com-
plex, non-transparent considerations, we do not consider general elasticity, but confines 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 $\varepsilon_{ij}$ may be expressed by the displacement gradient, [1]

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

The nonlinear product $u_{r,i} u_{r,j}$ is present in this expression. Therefore the deformation tensor $\varepsilon_{ij}$ 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 $\varepsilon_{ij}$. Second order elasticity is the simplest generalization of the linear elasticity. The expression for the elastic energy $\Phi$ (per unit volume in the stress-free state) takes into account the cubes, but neglects the fourth higher powers of strain tensor $\varepsilon_{ij}$. The elastic energy $\Phi$ reads

$$\Phi = \frac{1}{2} c_{ijklm} \varepsilon_{ij} \varepsilon_{km} + \frac{1}{6} c_{ijklmrs} \varepsilon_{ij} \varepsilon_{km} \varepsilon_{rs}. \tag{1.2}$$

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 $c_{ijklm}$ is the tensor of second order elastic constants and $c_{ijklmrs}$ 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 $\varepsilon_{ij}$ it may be assumed that $c_{ijklm} = c_{kmlij}$ and $c_{ijklmrs} = c_{kmrij}$ = $c_{ijrskm}$. Since $\varepsilon_{ij}$ is symmetric, it may be assumed without loosing the generality that the constants satisfy the relations $c_{ijklm} = c_{jiklm}$ and $c_{ijklmrs} = c_{jikmrs}$. 

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

\begin{equation}
  c_{ijkl} = c_{kl ij} = c_{jikl},
\end{equation}

\begin{equation}
  c_{ijklmrs} = c_{kmlsij} = c_{jirskm} = c_{jirskm}.
\end{equation}

Symmetry of the crystal results in additional symmetries. As mentioned above, the second order elastic constants $c_{ijkl}$ 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 $c_{ijkl}$ and 729 constants $c_{ijklmrs}$ 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 $\Phi$ with respect to the deformation $\varepsilon_{ij}$

\begin{equation}
  H_{ij} = \frac{\partial \Phi}{\partial \varepsilon_{ij}} + \frac{\partial \Phi}{\partial \varepsilon_{ji}}.
\end{equation}

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

\begin{equation}
  \frac{\partial \Phi}{\partial \varepsilon_{ij}} = c_{ijkl} \varepsilon_{km} + \frac{1}{2} c_{ijklmrs} \varepsilon_{km} \varepsilon_{rs},
\end{equation}

and further

\begin{equation}
  H_{ij} = 2c_{ijkl} \varepsilon_{km} + c_{ijklmrs} \varepsilon_{km} \varepsilon_{rs}.
\end{equation}

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

\begin{equation}
  2\tau_{ij} = H_{ij} + H_{ir}u_{i,r}.
\end{equation}

The stress tensor $\tau_{ij}$ 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 $\tau_{ij}$ 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

\[
k_i k_i = 1, \quad n_i n_i = 1, \quad k_i n_i = 0.
\]

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 shear reads

\[
u_i(x_r) = \nu k_i n_r x_r,
\]

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

\[
2\varepsilon_{ij} = \nu (k_i n_j + k_j n_i) + \nu^2 n_i n_j.
\]

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:

\[
\tau_{ij} = \nu c_{ijpq} k_p n_q
\]

\[
+ \nu^2 \left( \frac{1}{2} c_{ijpqrs} k_p k_r n_q n_s + \frac{1}{2} c_{ijpq} n_p n_q + c_{impq} k_j k_p n_m n_q \right).
\]

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

\[
t_j = \nu c_{ijpq} k_p n_i n_q
\]

\[
+ \nu^2 \left( \frac{1}{2} c_{ijpqrs} k_p k_r n_i n_q n_s + \frac{1}{2} c_{ijpq} n_i n_p n_q + k_j c_{impq} k_p n_j n_m n_q \right).
\]

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 \( n_i \).
\[ b_i = \varepsilon_{irs} k_r n_s, \]

where \( \varepsilon_{irs} \) 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 \( b_i \)

\[ s_k = t_j k_j, \quad s_n = t_j n_j, \quad s_b = t_j b_j. \]

In accord with the above relations there hold the relations

\[ s_k = \nu s_{k1} + \nu^2 (s_{k2} + s_{k3}), \]

\[ s_n = \nu s_{n1} + \nu^2 (s_{n2} + s_{n3}), \]

\[ s_b = \nu s_{b1} + \nu^2 (s_{b2} + s_{b3}), \]

where

\[ s_{k1} = c_{ijpq} k_i n_j k_p n_q, \]

\[ s_{k2} = \frac{3}{2} c_{ijpq} k_i n_j k_p n_q, \]

\[ s_{k3} = \frac{1}{2} c_{ijpqrs} k_i n_j k_p n_q k_r n_s. \]

\[ s_{n1} = c_{ijpq} n_i n_j k_p n_q, \]

\[ s_{n2} = \frac{1}{2} c_{ijpq} n_i n_j n_p n_q, \]

\[ s_{n3} = \frac{1}{2} c_{ijpqrs} n_i n_j k_p n_q k_r n_s. \]

\[ s_{b1} = c_{ijpq} b_i n_j k_p n_q, \]

\[ s_{b2} = \frac{3}{2} c_{ijpq} b_i n_j k_p n_q, \]

\[ s_{b3} = \frac{1}{2} c_{ijpqrs} b_i n_j k_p n_q k_r n_s. \]

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 \( \nu \) and a part proportional to the squared amount of shear \( \nu^2 \). 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 \( \nu \) the first terms \( s_{k1}, s_{n1}, s_{b1} \) in (1.17)–(1.19) are the leading terms. For other \( \nu \) 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 \( \nu \). Stiffness is equal to the sum

\[
(1.20) \quad s = s_{k1} + \nu(s_{k2} + s_{k3}).
\]

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

\[
s_{k1} = c_{ijpq}k_in_jk_pn_q,
\]

\[
s_{n1} = c_{ijpq}n_in_jk_pn_q,
\]

\[
s_{b1} = c_{ijpq}b_in_jk_pn_q.
\]

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 \((e_1 = \varepsilon_{11}, e_2 = \varepsilon_{22}, \ldots, e_4 = 2\varepsilon_{23}, \text{etc.})\) 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

\[
c_{1111} = c_{2222} = c_{3333} = h_{11},
\]

\[
c_{1122} = c_{1133} = c_{2233} = c_{2211} = c_{3311} = c_{3322} = h_{12},
\]

\[
c_{2323} = c_{2332} = c_{3223} = \ldots = c_{1212} = c_{1221} = h_{44}.
\]

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 \( s_{k_2}, s_{n_2} \) and \( s_{b_2} \) 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

\[
k_i^{(1)} = (0,1,0), \quad k_i^{(2)} = (0,1,1), \quad k_i^{(3)} = (0,1,1 + \sqrt{2}).
\]

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 \( s_{k_2}, s_{n_2} \) and \( s_{b_2} \) 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

\[
k_i^{(4)} = (1,-1,0), \quad k_i^{(5)} = (0,0,1), \quad k_i^{(6)} = (1,-1,\sqrt{2})
\]

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

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

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 \( k_i^{(1)}, k_i^{(2)}, \ldots, k_i^{(9)} \) 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 \( s_{k_1}, s_{n_1} \) and \( s_{b_1} \) 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>
<thead>
<tr>
<th>$n_i$</th>
<th>$k_i$</th>
<th>$h_{11}=1, h_{12}=0, h_{44}=0$</th>
<th>$h_{11}=0, h_{12}=1, h_{44}=0$</th>
<th>$h_{11}=0, h_{12}=0, h_{44}=1$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$s_{k1}$</td>
<td>$s_{n1}$</td>
<td>$s_{b1}$</td>
</tr>
<tr>
<td>(1,0,0)</td>
<td>$k_i^{(1)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(2)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(3)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(1,1,0)</td>
<td>$k_i^{(4)}$</td>
<td>0.500</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(5)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(6)}$</td>
<td>0.250</td>
<td>0</td>
<td>-0.250</td>
</tr>
<tr>
<td>(1,1,1)</td>
<td>$k_i^{(7)}$</td>
<td>0.333</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(8)}$</td>
<td>0.333</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(9)}$</td>
<td>0.333</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Table 2. Coefficients $s_{n_2}$ for $n_i=(1,0,0)$, $n_i=(1,1,0)$ and $n_i=(1,1,1)$.

<table>
<thead>
<tr>
<th>$n_i$</th>
<th>$k_i$</th>
<th>$h_{11}=1$</th>
<th>$h_{12}=1$</th>
<th>$h_{44}=1$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$s_{k_2}$</td>
<td>$s_{n_2}$</td>
<td>$s_{b_2}$</td>
</tr>
<tr>
<td>(1,0,0)</td>
<td>$k_i^{(1)}$</td>
<td>0</td>
<td>.500</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(2)}$</td>
<td>0</td>
<td>.500</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(3)}$</td>
<td>0</td>
<td>.500</td>
<td>0</td>
</tr>
<tr>
<td>(1,1,0)</td>
<td>$k_i^{(4)}$</td>
<td>.750</td>
<td>.250</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(5)}$</td>
<td>0</td>
<td>.250</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(6)}$</td>
<td>.375</td>
<td>.250</td>
<td>-.125</td>
</tr>
<tr>
<td>(1,1,1)</td>
<td>$k_i^{(7)}$</td>
<td>.500</td>
<td>.167</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(8)}$</td>
<td>.500</td>
<td>.167</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_i^{(9)}$</td>
<td>.500</td>
<td>.167</td>
<td>0</td>
</tr>
</tbody>
</table>
$n_i=(1,0,0)$ 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 $\nu^2$. 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

\[(3.1) \hspace{1cm} (k_1, k_2, k_3) \Rightarrow (-k_1, -k_2, -k_3)\]

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 $h_{111}=1$, $h_{112}=1$, $h_{123}=1$.

<table>
<thead>
<tr>
<th>$n_i$</th>
<th>$k_i$</th>
<th>$h_{111}=1$, other $h_{\alpha\beta\gamma}=0$</th>
<th>$h_{112}=1$, other $h_{\alpha\beta\gamma}=0$</th>
<th>$h_{123}=1$, other $h_{\alpha\beta\gamma}=0$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$s_{k3}$</td>
<td>$s_{n3}$</td>
<td>$s_{b3}$</td>
</tr>
<tr>
<td>(1,0,0)</td>
<td>$k_{(1)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_{(2)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_{(3)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(1,1,0)</td>
<td>$k_{(4)}$</td>
<td>0</td>
<td>.125</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_{(5)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_{(6)}$</td>
<td>0</td>
<td>.062</td>
<td>0</td>
</tr>
<tr>
<td>(1,1,1)</td>
<td>$k_{(7)}$</td>
<td>.039</td>
<td>.056</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$k_{(8)}$</td>
<td>0</td>
<td>.056</td>
<td>-.039</td>
</tr>
<tr>
<td></td>
<td>$k_{(9)}$</td>
<td>.028</td>
<td>.056</td>
<td>-.028</td>
</tr>
<tr>
<td>( n_i )</td>
<td>( k_1 )</td>
<td>( k_{12} )</td>
<td>( k_{23} )</td>
<td>( k_{34} )</td>
</tr>
<tr>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>(1,0,0)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(1,1,0)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>(1,1,1)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 4. Coefficients \( s_{k3}, s_{n3}, s_{k8} \) for \( h_{144}=1, h_{455}=1, h_{466}=1 \).
\[(n_1, n_2, n_3) \Rightarrow (-n_1, n_2, n_3) \quad \text{and} \quad (k_1, k_2, k_3) \Rightarrow (-k_1, k_2, k_3),\]

\[(n_1, n_2, n_3) \Rightarrow (n_1, -n_2, n_3) \quad \text{and} \quad (k_1, k_2, k_3) \Rightarrow (k_1, -k_2, k_3),\]

\[(n_1, n_2, n_3) \Rightarrow (n_1, n_2, -n_3) \quad \text{and} \quad (k_1, k_2, k_3) \Rightarrow (k_1, k_2, -k_3).\]

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

\[n_1 = \sin \vartheta \cos \varphi,\]

\[n_2 = \sin \vartheta \sin \varphi,\]

\[n_3 = \cos \vartheta;\]

\[k_1 = \cos \psi \cos \vartheta \cos \varphi - \sin \psi \sin \varphi,\]

\[k_2 = \cos \psi \cos \vartheta \sin \varphi + \sin \psi \cos \varphi,\]

\[k_3 = -\cos \psi \sin \vartheta.\]

The two angles \(\vartheta\) and \(\varphi\) 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 \(\psi\), together with \(\vartheta\) and \(\varphi\) 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

\[b_1 = -\sin \psi \cos \vartheta \cos \varphi - \cos \psi \sin \varphi,\]

\[b_2 = -\sin \psi \cos \vartheta \sin \varphi + \cos \psi \cos \varphi,\]

\[b_3 = \sin \psi \sin \vartheta.\]

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 \(\vartheta, \varphi, \psi\). For
arbitrary \((\vartheta, \varphi, \psi)\) 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 \((\vartheta, \varphi, \psi)\) by other values results in reflection in the shearing planes and shearing directions in the coordinate planes

\[
(n_1, n_2, n_3), (k_1, k_2, k_3) \Rightarrow (n_1, n_2, n_3), (k_1, k_2, k_3)
\]
\[
\text{if } (\vartheta, \varphi, \psi) \Rightarrow (\vartheta, \pi - \varphi, -\psi),
\]
\[
(4.4) \quad (n_1, n_2, n_3), (k_1, k_2, k_3) \Rightarrow (n_1, -n_2, n_3), (k_1, -k_2, k_3)
\]
\[
\text{if } (\vartheta, \varphi, \psi) \Rightarrow (\vartheta, -\varphi, -\psi),
\]
\[
(n_1, n_2, n_3), (k_1, k_2, k_3) \Rightarrow (n_1, n_2, -n_3), (k_1, k_2, -k_3)
\]
\[
\text{if } (\vartheta, \varphi, \psi) \Rightarrow (\vartheta, \pi - \varphi, -\psi).
\]

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 \(\vartheta\), \(\varphi\) and \(\psi\). 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

\[
h_{11} = 169 \text{ GPa}, \quad h_{12} = 122 \text{ GPa}, \quad h_{44} = 73.5 \text{ GPa},
\]
\[
(4.5)
\]
\[
h_{111} = -1350 \text{ GPa}, \quad h_{112} = -800 \text{ GPa}, \quad h_{123} = -120 \text{ GPa},
\]
\[
h_{144} = -66 \text{ GPa}, \quad h_{155} = -720 \text{ GPa}, \quad h_{456} = -32 \text{ GPa}.
\]
\[
(4.6)
\]

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 \((k_1, k_2, k_3)\)

\[
(n_1, n_2, n_3), (k_1, k_2, k_3) \Rightarrow (n_2, n_1, n_3), (k_2, k_1, k_3),
\]
\[
(n_1, n_2, n_3), (k_1, k_2, k_3) \Rightarrow (n_1, n_3, n_2), (k_1, k_3, k_2),
\]
\[
(n_1, n_2, n_3), (k_1, k_2, k_3) \Rightarrow (n_3, n_2, n_1), (k_3, k_2, k_1),
\]
do not change the properties of the crystal, i.e. the values of $s_{k1}, s_{n1}, s_{b1} s_{k1}, \ldots, s_{b3}$.

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 $n_3, n_4 > 0$. 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>
<thead>
<tr>
<th></th>
<th>Value</th>
<th>$\theta, \varphi, \psi$</th>
<th>$n_i$</th>
<th>$k_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$s_{k1}$</td>
<td>max</td>
<td>75.30 (.393,0.1571)</td>
<td>(.383,0.924)</td>
<td>(0,1,0)</td>
</tr>
<tr>
<td></td>
<td>m/m</td>
<td>36.45 (.785,.785)</td>
<td>(.500,.500,.707)</td>
<td>(.500,.500,.707)</td>
</tr>
<tr>
<td></td>
<td>min</td>
<td>23.50 (1.571,785,1.571)</td>
<td>(.707,.707)</td>
<td>(-.707,.707)</td>
</tr>
<tr>
<td>$s_{n1}$</td>
<td>max</td>
<td>29.06 (1.261,326,2.306)</td>
<td>(.902,305,305)</td>
<td>(-.431,.631,.646)</td>
</tr>
<tr>
<td></td>
<td>m/m</td>
<td>0 (1,0,0)</td>
<td>(-.500,.707,.500)</td>
<td>(-.500,.707,.500)</td>
</tr>
<tr>
<td></td>
<td>min</td>
<td>-29.06 (1.263,1245,841)</td>
<td>(.305,902,305)</td>
<td>(-.638,.431,.638)</td>
</tr>
<tr>
<td>$s_{b1}$</td>
<td>max</td>
<td>25.90 (-.785,3142,.785)</td>
<td>(.707,.707)</td>
<td>(-.500,.707,.500)</td>
</tr>
<tr>
<td></td>
<td>m/m</td>
<td>0* (1.571,1.571)</td>
<td>(1,0,0)</td>
<td>(0,1,0)</td>
</tr>
<tr>
<td></td>
<td>min</td>
<td>-25.90 (1.571,785,785)</td>
<td>(.707,.707)</td>
<td>(-.500,.500,.707)</td>
</tr>
</tbody>
</table>

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 $\psi$. For $\psi = \pi/2$ the normal to the shearing plane and the shearing direction coincide with the coordinate 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 $\psi$.

<table>
<thead>
<tr>
<th></th>
<th>Value</th>
<th>$\theta, \varphi, \psi$</th>
<th>$n_i$</th>
<th>$k_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$s_{k2}$</td>
<td>max</td>
<td>112.95 (0,758,0)</td>
<td>(0,0,1)</td>
<td>(.707,.707)</td>
</tr>
<tr>
<td></td>
<td>m/m</td>
<td>54.68 (.785,.785)</td>
<td>(.500,.500,.707)</td>
<td>(.500,.500,.707)</td>
</tr>
<tr>
<td></td>
<td>min</td>
<td>35.25 (.785,0,0)</td>
<td>(.707,.707)</td>
<td>(.707,.707)</td>
</tr>
<tr>
<td>$s_{n2}$</td>
<td>max</td>
<td>119.03 (.955,785,732)</td>
<td>(.577,577,577)</td>
<td>(-.169,776,.607)</td>
</tr>
<tr>
<td></td>
<td>m/m</td>
<td>110.40 (.785,0,0)</td>
<td>(.707,.707)</td>
<td>(.707,.707)</td>
</tr>
<tr>
<td></td>
<td>min</td>
<td>84.50* (.785,0,0)</td>
<td>(0,0,1)</td>
<td>(.707,.707)</td>
</tr>
<tr>
<td>$s_{b2}$</td>
<td>max</td>
<td>38.85 (.785,1571,785)</td>
<td>(.707,.707)</td>
<td>(-.707,500,.500)</td>
</tr>
<tr>
<td></td>
<td>min</td>
<td>-38.85 (1.571,785,785)</td>
<td>(.707,.707)</td>
<td>(-.500,.500,.707)</td>
</tr>
</tbody>
</table>

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>
<thead>
<tr>
<th>$s_{k3}$</th>
<th>max</th>
<th>160.59</th>
<th>(1.047, .615, .956)</th>
<th>(0.707, .500, .500)</th>
<th>(0.707, -.500, -.500)</th>
</tr>
</thead>
<tbody>
<tr>
<td>max</td>
<td>64.82</td>
<td>(228, .785, 0)</td>
<td>(159, .159, .974)</td>
<td>(0.689, .689, -.226)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-64.82</td>
<td>(-228, .927, 0)</td>
<td>(150, .150, .974)</td>
<td>(-0.689, -.689, .228)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-160.59</td>
<td>(.785, .785, 0)</td>
<td>(.500, .500, .707)</td>
<td>(.500, .500, -.707)</td>
<td></td>
</tr>
<tr>
<td>$s_{n3}$</td>
<td>max</td>
<td>-68.75</td>
<td>(.785, 0, 0)</td>
<td>(.707, 0, 707)</td>
<td>(.707, 0, -.707)</td>
</tr>
<tr>
<td>max</td>
<td>-109.69</td>
<td>(.555, .785, 0)</td>
<td>(.372, .372, .850)</td>
<td>(.601, .601, -.527)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-360.0</td>
<td>(0, .785, 0)</td>
<td>(0, 0, 1)</td>
<td>(.707, .707, 0)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-395.15</td>
<td>(1.211, .385, .715)</td>
<td>(.868, .352, .352)</td>
<td>(0, -.707, 0)</td>
<td></td>
</tr>
<tr>
<td>$S_{b3}$</td>
<td>max</td>
<td>125.24</td>
<td>(.887, .952, .423)</td>
<td>(.450, .632, .632)</td>
<td>(.707, .707, 0)</td>
</tr>
<tr>
<td>max</td>
<td>73.75</td>
<td>(-.393, .3142, 1.571)</td>
<td>(.383, 0, .924)</td>
<td>(0, -.10)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-73.75</td>
<td>(.393, 0, 1.571)</td>
<td>(.383, 0, .924)</td>
<td>(0, 1.0)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-125.24</td>
<td>(1.104, .785, 1.571)</td>
<td>(.632, .632, .450)</td>
<td>(-.707, .707, 0)</td>
<td></td>
</tr>
</tbody>
</table>

Since both $s_{k2}$ and $s_{k3}$ contribute to the stress proportionally to $\nu^2$, 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>
<thead>
<tr>
<th>$s_{k2} + s_{k3}$</th>
<th>max</th>
<th>215.27</th>
<th>(1.047, .615, -.956)</th>
<th>(0.707, .500, .500)</th>
<th>(0.707, -.500, -.500)</th>
</tr>
</thead>
<tbody>
<tr>
<td>max</td>
<td>167.72</td>
<td>(.201, .785, 0)</td>
<td>(.141, .141, .980)</td>
<td>(.693, .693, -.200)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-.230, 3.824, 125</td>
<td>(.177, .144, .974)</td>
<td>(-.671, -.706, .23)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>35.45</td>
<td>(-.258, 3.903, 0.26)</td>
<td>(.185, .176, .967)</td>
<td>(-.684, -.684, .25)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-105.92</td>
<td>(.785, .785, 0)</td>
<td>(.500, .500, .707)</td>
<td>(.500, .500, -.707)</td>
<td></td>
</tr>
<tr>
<td>$s_{n2} + s_{n3}$</td>
<td>max</td>
<td>41.65</td>
<td>(.785, 0, 0)</td>
<td>(.707, 0, 707)</td>
<td>(.707, 0, -.707)</td>
</tr>
<tr>
<td>max</td>
<td>-2.05</td>
<td>(.569, .785, 0)</td>
<td>(.381, .381, .841)</td>
<td>(.596, .596, -.538)</td>
<td></td>
</tr>
<tr>
<td>max</td>
<td>-102.10</td>
<td>(.157, .785, 0)</td>
<td>(.707, 0, 707)</td>
<td>(0, 1.000)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-275.50</td>
<td>(0, .785, 0)</td>
<td>(0, 0, 1)</td>
<td>(.707, .707, 0)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-291.9</td>
<td>(1.264, .323, .731)</td>
<td>(.904, .302, .302)</td>
<td>(0, .707, -.707)</td>
<td></td>
</tr>
<tr>
<td>$s_{b2} + s_{b3}$</td>
<td>max</td>
<td>126.35</td>
<td>(.861, .938, .462)</td>
<td>(.448, .611, .652)</td>
<td>(.014, .734, -.67)</td>
</tr>
<tr>
<td>max</td>
<td>75.79</td>
<td>(-.401, 3.202, 1.435)</td>
<td>(.024, .921, .389)</td>
<td>(.996, .054, -.06)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-53.2</td>
<td>(-.291, 4.137, -.785)</td>
<td>(.156, .611, .448)</td>
<td>(-.962, -.184, 208)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-75.79</td>
<td>(.401, 1.512, 1.704)</td>
<td>(.023, .390, .921)</td>
<td>(-.997, -.064, .052)</td>
<td></td>
</tr>
<tr>
<td>min</td>
<td>-126.35</td>
<td>(1.060, .753, 1.553)</td>
<td>(.652, .611, .448)</td>
<td>(.678, .735, -.016)</td>
<td></td>
</tr>
</tbody>
</table>

The angles $(\vartheta, \varphi, \psi)$ make easier the computations. Obviously, instead of the angles $(\vartheta, \varphi, \psi)$ 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 (0.500, 0.500, 0.707) 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. (0.652, 0.611, 0.448) 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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References


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