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Number of longitudinal normals and degenerate directions for triclinic and monoclinic media

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Abstract. We solved the problem of finding longitudinal acoustic directions of monoclinic media using the eliminant method. By extending Khatkevich's approach and using the Bezout theorem, we proved that the number of longitudinal normals for mechanically stable monoclinic media can not be larger than 13. Both longitudinal normals (n_1, n_2, n_3) lying in and out of plane perpendicular to the two-fold axis $(n_3 \neq 0)$ of monoclinic media are considered. Closed-form equations for ratios $x = n_1/n_3$ $y = n_2/n_3$ are derived and exactly solved by the eliminant method. With the help of this method, we show that in the case of the CDP (CsH_2PO_4) crystal, the number of longitudinal normals equals three. Their components are given. For media of higher symmetries (rhombic, trigonal, tetragonal, hexagonal and cubic), our approach yields well-known results obtained mainly by Borgnis and Khatkevich. For triclinic elastic media, we proved that the number of degenerate directions can not be greater than 132.

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1 Introduction

Longitudinal normals are directions in anisotropic elastic media, along which the pure longitudinal and pure transverse waves can propagate. The number of these axes and their spatial directions are of importance for the exact determination of elastic constants of media. For this reason they were investigated for a number of years [1–10].

Acoustic waves with at least two phase velocities equal propagate in so called degenerate directions. Please note that directions along which waves with at least two phase velocities equal propagate are also sometimes called *acoustic axes* or singularities [8]. However in this article we will use the term *degenerate direction*.

Khatkevich developed a method of establishing the longitudinal normals and degenerate directions [3,9,10]. He estimated the number of longitudinal normals and degenerate directions for elastic media of all symmetries, except triclinic ones. Helbig [10] studied triclinic media and found that the number of longitudinal normals is equal to 13.

In a previous paper one of us applied the method of eliminants to the problem of establishing longitudinal normals for triclinic media [11]. In particular, it was shown that for triclinic media, the number of longitudinal normals is not greater than 16. Two univariate polynomial equations were obtained, which generally can be solved only numerically. An example, namely the oligoclase crystal, was considered.

Our method can be treated as an extension of the Khatkevich method. Namely, to the set of equations obtained from the condition of existence of longitudinal axes, we apply the standard and powerful method of eliminants [12]. In the Khatkevich approach, this condition is transformed to the set of rather complicated vectorial relations. The proposed method of determination of longitudinal normals can be used to assist in identifying the crystallographic symmetry in situations where other methods (*e.g.* X-ray difractometry) have led to uncertainties or ambiguities [13].

In this paper we apply the method of eliminants to monoclinic elastic media. Equations determining these axes in the case of media more symmetric than monoclinic and triclinic are well-known, and we checked that our methods give the same results [14]. The eliminant method is based on theorems of algebra of polynomials. For this reason, it is well suited for construction of algorithms of numerical calculations. This allows us to modify our program, the algorithm of which was based on the Euler rotations [15]. Designing our previous program, we used an observation made by Fedorov [8] that in the coordinate system in which the Z axis is directed along a longitudinal normal the elastic constants C_{35}, C_{45} have to vanish. Consequently, we rotated the sample until these components of $\hat{C}$ vanished, *i.e.*, we considered all similarity transformations generated by the Euler rotations,

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which yield a matrix $\hat{C}$ with $C_{35} = 0$, $C_{45} = 0$. In the next step, we checked which of the longitudinal normals are the symmetry axes [15]. The eliminant method provides us with a more flexible and systematic tool of searching for longitudinal normals.

Furthermore, we consider here another interesting and not yet solved problem, namely in the case of triclinic media, we look for the number of degenerate directions. We proved that their number can not be greater than 132.

2 Equations for longitudinal normals for elastic media of an arbitrary elastic symmetry

The elastic and acoustic properties of crystalline bodies are defined by the mass density ρ and a set of elements $C_{\alpha\mu,\beta\nu}$ $(\alpha, \beta, \mu, \nu = 1, 2, 3)$ of a matrix $\hat{C}$, representing the tensor of elastic constants in a chosen laboratory coordinate system. Assume that a plane wave propagates in the direction $\mathbf{n} = (n_1, n_2, n_3)$. In the chosen coordinate system, the acoustical tensor $\tilde{\Gamma}(\mathbf{n})$ is represented by the matrix $\hat{\Gamma}(\mathbf{n})$, with elements

$$\left[\hat{\Gamma}(\mathbf{n})\right]_{\alpha\beta} = \Gamma_{\alpha\beta}(\mathbf{n}) = \rho^{-1} \sum_{\mu,\nu=1}^{3} n_\mu \, C_{\alpha\mu,\beta\nu} \, n_\nu. \quad (1)$$

Along a longitudinal normal $\mathbf{n}_l$, one pure longitudinal and two pure transverse waves propagate [8]. This means that the vector of propagation $\mathbf{n}_l$ is the eigenvector of the acoustical tensor $\tilde{\Gamma}$ [9]

$$\Gamma(\mathbf{n}_l)\mathbf{n}_l = c^2 \, \mathbf{n}_l, \quad (2a)$$

or for components of $\mathbf{n}_l$

$$\left[n_l^{(1)}, n_l^{(2)}, n_l^{(3)}\right] = \left[\frac{1}{c^2}\sum_{j=1}^{3}\Gamma_{1j}n_l^{(j)}, \frac{1}{c^2}\sum_{j=1}^{3}\Gamma_{2j}n_l^{(j)}, \frac{1}{c^2}\sum_{j=1}^{3}\Gamma_{3j}n_l^{(j)}\right], \quad (2b\text{-}d)$$

where c is a positive number. Equations (2b–d) imply that

$$\frac{\sum_{j=1}^{3}\Gamma_{1j}n_l^{(j)}}{\sum_{j=1}^{3}\Gamma_{3j}n_l^{(j)}} = \frac{n_l^{(1)}}{n_l^{(3)}}, \quad \frac{\sum_{j=1}^{3}\Gamma_{2j}n_l^{(j)}}{\sum_{j=1}^{3}\Gamma_{3j}n_l^{(j)}} = \frac{n_l^{(2)}}{n_l^{(3)}} \cdot$$

By making substitutions $x = n_1/n_3$, $y = n_2/n_3$ $(n_3 \neq 0)$, the above set of equations for triclinic media takes the following form:

$$P_{tricl}^{(1)}(x, y) = A_0^{(t)}(y) + A_1^{(t)}(y)x + A_2^{(t)}(y)x^2 + A_3^{(t)}(y)x^3 + A_4^{(t)}(y)x^4, \quad (3a)$$

$$P_{tricl}^{(2)}(x, y) = B_0^{(t)}(y) + B_1^{(t)}(y)x + B_2^{(t)}(y)x^2 + B_3^{(t)}(y)x^3, \quad (3b)$$

where $A_\alpha(y)$, $B_\alpha(y)$ $(\alpha = 0, 1, 2, 3)$ are polynomials of a variable y

$$\begin{aligned}
A_0^{(t)}(y) &= C_{35} + (2C_{45} + C_{36})y + (2C_{46} + C_{25})y^2 + C_{26}y^3,\\
A_1^{(t)}(y) &= (C_{13} + 2C_{55} - C_{33}) + (4C_{56} + 2C_{14} + 3C_{34})y\\
&\quad + (2C_{66} + C_{12} - 2C_{44} - C_{23})y^2 - C_{24}y^3,\\
A_2^{(t)}(y) &= (3C_{15} - 3C_{35}) + (3C_{16} - 4C_{45} - 2C_{36})y\\
&\quad - (2C_{46} + C_{25})y^2,\\
A_3^{(t)}(y) &= (C_{11} - C_{13} - 2C_{55}) - (2C_{56} + C_{14})y,\\
A_4^{(t)}(y) &= -C_{15}.
\end{aligned} \quad (4a)$$

$$\begin{aligned}
B_0^{(t)}(y) &= C_{34} + (2C_{44} + C_{23} - C_{33})y + (3C_{24} - 3C_{34})y^2\\
&\quad + (C_{22} - 2C_{44} - C_{23})y^3 - C_{24}y^4,\\
B_1^{(t)}(y) &= (2C_{45} + C_{36}) + (2C_{25} + 4C_{46} - 3C_{35})y\\
&\quad + (3C_{26} - 2C_{36} - 4C_{45})y^2 - (2C_{46} + C_{25})y^3,\\
B_2^{(t)}(y) &= (2C_{56} + C_{14}) + (C_{12} - 2C_{55} - C_{13} + 2C_{66})y\\
&\quad - (2C_{56} + C_{14})y^2,\\
B_3^{(t)}(y) &= C_{16} - C_{15}y.
\end{aligned} \quad (4b)$$

One can obtain polynomials $P_1(x, y)$, $P_2(x, y)$ for media of higher symmetry by reducing accordingly the number of non-vanishing independent elastic constants.

We shall solve the set of bivariate polynomial equations

$$P_{tricl}^{(1)}(x, y) = 0, \quad P_{tricl}^{(2)}(x, y) = 0, \quad (5a, b)$$

by the method of eliminants [12]. Now we briefly describe this method in the case of general case of triclinic media. The eliminant $E_{tricl}(y)$ of equations (5) is the following determinant:

$$E_{tricl}(y) = \begin{vmatrix}
A_4(y) & A_3(y) & A_2(y) & A_1(y) & A_0(y) & 0 & 0\\
0 & A_4(y) & A_3(y) & A_2(y) & A_1(y) & A_0(y) & 0\\
0 & 0 & A_4(y) & A_3(y) & A_2(y) & A_1(y) & A_0(y)\\
B_3(y) & B_2(y) & B_1(y) & B_0(y) & 0 & 0 & 0\\
0 & B_3(y) & B_2(y) & B_1(y) & B_0(y) & 0 & 0\\
0 & 0 & B_3(y) & B_2(y) & B_1(y) & B_0(y) & 0\\
0 & 0 & 0 & B_3(y) & B_2(y) & B_1(y) & B_0(y)
\end{vmatrix}. \quad (6)$$

The necessary condition for the existence of solutions of equations (5a, b) is that

$$E_{tricl}(y) = 0. \quad (7)$$

The order of equation (7) is generally higher than 4, and therefore it can only be solved numerically. After substitution of the roots of the eliminant to equations (5a, b), we obtain a pair of equations for x.

Clearly, we deal with two univariate polynomial equations. Assume that they are respectively of degree m and p, and that the number of their solutions is finite. The Bezout theorem states that the number of real solutions of this set can not be larger than the product $m \times p$.

3 Determination of number of degenerate directions for triclinic media

Denote the direction of degenerate direction by $\mathbf{n}_a$. We shall prove a lemma.

Lemma 1

If a continuous bivariable polynomial function $F(x, y)$ of the degree p defined on R^2 has finite number of zeros, then this number can not be larger than $p(p-1)$.

Proof: If in a set of values of $F(x, y)$ one can find at least one pair of numbers with different signs, then the equation

$$F(x, y) = 0, \tag{8}$$

has infinite number of roots. Indeed, if a continuous function $F(x, y)$ is negative for $(x_0^{(-)}, y_0^{(-)})$; then one can find a circular region $K-$ for which $F(x, y) < 0$. Similarly, if a continuous function $F(x, y)$ is positive for $(x_0^{(+)}, y_0^{(+)})$, then one can find a circular region $K+$ for which $F(x, y) > 0$. $K-$ and $K+$ are disjoint. One may find infinitely many intervals joining points of $K-$, $K+$. Since $F(x, y)$ is continuous on R^2, on each of these intervals a point exists for which F vanishes. Thus, equation (8) has infinitely many roots.

This means that if equation (8) has a finite number of roots, the continuous function $F(x, y)$ is nonnegative or nonpositive in R^2. Therefore, for each root of equation (8), $F(x, y)$ attains a local extremum. These roots can be found from conditions

$$F(x, y) = 0; \quad \partial F(x, y)/\partial x = 0. \tag{9a, b}$$

We obtained the set of two polynomial equations: (9a) is of the degree p, whereas (9b) at most of $(p-1)$ degree. Since we assumed that $F(x, y)$ has finite number of zeros, the set of bivariate polynomial equations has a finite number of solutions. From the Bezout theorem it follows that their number cannot be greater than $p(p-1)$. Therefore, we have proven the lemma.

Consider an elastic wave propagating in a direction $\mathbf{n}$. In the chosen Cartesian coordinate system, $\mathbf{n}$ has components n_1, n_2, n_3 and the phase velocities are eigenvalues of the suitable propagation matrix $\hat{\Gamma}(n_1, n_2, n_3)$. If $\mathbf{n}$ is a degenerate direction, then at least two phase velocities $c_j(\mathbf{n})$ $(j = 0, 1, 2)$ are equal. The characteristic equation for $c_j(\mathbf{n})$ has the following form:

$$\begin{aligned} &c^3 - \left[\Gamma_{11}(\mathbf{n}) + \Gamma_{22}(\mathbf{n}) + \Gamma_{33}(\mathbf{n})\right]c^2 + \left[\Gamma_{11}(\mathbf{n})\Gamma_{22}(\mathbf{n})\right. \\ &\left.+\Gamma_{11}(\mathbf{n})\Gamma_{33}(\mathbf{n}) + \Gamma_{22}(\mathbf{n})\Gamma_{33}(\mathbf{n}) - \Gamma_{23}^2(\mathbf{n}) - \Gamma_{12}^2(\mathbf{n}) - \Gamma_{13}^2(\mathbf{n})\right]c \\ &+ \left[\Gamma_{11}(\mathbf{n})\Gamma_{23}^2(\mathbf{n}) + \Gamma_{33}(\mathbf{n})\Gamma_{12}^2(\mathbf{n}) + \Gamma_{22}(\mathbf{n})\Gamma_{13}^2(\mathbf{n})\right. \\ &\left.- \Gamma_{11}(\mathbf{n})\Gamma_{22}(\mathbf{n})\Gamma_{33}(\mathbf{n}) - 2\Gamma_{12}(\mathbf{n})\Gamma_{13}(\mathbf{n})\Gamma_{23}(\mathbf{n})\right] = 0. \end{aligned} \tag{10}$$

Equation (10) has a double root for $\mathbf{n}$ directed along each $\mathbf{n}_a$. A cubic equation has double root, if, and only if, its discriminant $\Delta(\mathbf{n})$ vanishes.

For equation (10) the discriminant reads

$$\Delta(n_1, n_2, n_3) = q^2(n_1, n_2, n_3) + \frac{4}{27}p^3(n_1, n_2, n_3), \tag{11}$$

where

$$\begin{aligned} q(n_1, n_2, n_3) = &(\Gamma_{11}\Gamma_{22}\Gamma_{33} - \Gamma_{11}\Gamma_{23}^2 - \Gamma_{33}\Gamma_{12}^2 + 2\Gamma_{12}\Gamma_{13}\Gamma_{23} \\ &- \Gamma_{22}\Gamma_{13}^2) - 2(\Gamma_{11} + \Gamma_{22} + \Gamma_{33})^3/27 - (\Gamma_{11} + \Gamma_{22} + \Gamma_{33}) \\ &\times \left[\Gamma_{23}^2 + \Gamma_{12}^2 + \Gamma_{13}^2 - \Gamma_{11}\Gamma_{22} - \Gamma_{11}\Gamma_{33} - \Gamma_{22}\Gamma_{33}\right]/3, \end{aligned} \tag{12a}$$

and

$$\begin{aligned} p(n_1, n_2, n_3) = &-(\Gamma_{11} + \Gamma_{22} + \Gamma_{33})^2/3 \\ &- (\Gamma_{23}^2 + \Gamma_{12}^2 + \Gamma_{13}^2 - \Gamma_{11}\Gamma_{22} - \Gamma_{11}\Gamma_{33} - \Gamma_{22}\Gamma_{33}). \end{aligned} \tag{12b}$$

Each element of $\hat{\Gamma}(n_1, n_2, n_3)$ is a homogeneous polynomial function of variables n_1, n_2, n_3 of the second order. On the other hand, the discriminant (11) is a homogeneous function of variables $\Gamma_{ij}(n_1, n_2, n_3)$ $(i, j = 1, 2, 3)$ of the sixth order. Hence, $\Delta(\mathbf{n})$ is a homogeneous function of n_1, n_2, n_3 of the twelfth order. If the number of degenerate directions is finite, then one can find a plane without degenerate directions. One may choose a Cartesian coordinate system where this plane is perpendicular to z axis. In this coordinate system, $n_3 \neq 0$. In variables $x = n_1/n_3$, $y = n_2/n_3$, the discriminant $\Delta(\mathbf{n})$ is a function of x and y of the twelfth order ($m = 12$). From the *Lemma 1*, it follows that the number of degenerate directions of an elastic medium cannot be greater than $11 \times 12 = 132$.

4 Monoclinic media: Longitudinal normals lying outside of the symmetry plane

Elastic media which contain only one symmetry axis of the second order C_2 are called monoclinic media. They also contain one symmetry plane perpendicular to this symmetry axis. For monoclinic media, $C_{14} = C_{24} = C_{34} = C_{15} = C_{25} = C_{35} = C_{46} = C_{56} = 0$. Longitudinal directions of monoclinic media were investigated by Khatkevich [9]. He stated that media with this symmetry can contain longitudinal axes the number of which vary from 3 to 17. For monoclinic media, one has

$$A_0^{(m)}(y) = (2C_{45} + C_{36})y + C_{26}y^3,$$
$$A_1^{(m)}(y) = (C_{13} + 2C_{55} - C_{33}) + (2C_{66} - 2C_{44} - C_{23} + C_{12})y^2,$$
$$A_2^{(m)}(y) = (3C_{16} - 4C_{45} - 2C_{36})y,$$
$$A_3^{(m)}(y) = (C_{11} - 2C_{55} - C_{13}), \qquad (13a\text{-}d)$$

$$B_0^{(m)}(y) = (2C_{44} + C_{23} - C_{33})y + (C_{22} - C_{23} - 2C_{44})y^3,$$
$$B_1^{(m)}(y) = (2C_{45} + C_{36}) + (3C_{26} - 2C_{36} - 4C_{45})y^2,$$
$$B_2^{(m)}(y) = (2C_{66} + C_{12} - C_{13} - 2C_{55})y,$$
$$B_3^{(m)}(y) = C_{16}. \qquad (14a\text{-}d)$$

Two equations

$$P^{(1)}_{monocl}(x, y) = 0, \quad P^{(2)}_{monocl}(x, y) = 0, \qquad (15a, b)$$

have solutions if

$$E_{monocl}(y) = 0. \qquad (16)$$

The Bezout theorem applied to equations (15) implies that maximal number of longitudinal normals which lie outside the plane $n_3 = 0$ equals 9. Fedorov has proven that each symmetry axis is also the longitudinal normal. Thus, in the considered case, the two-fold symmetry axis is a longitudinal normal. The existence of a twofold symmetry axis entails that to each longitudinal normal which lies out of the plane OXY $(n_l^{(1)}, n_l^{(2)}, n_l^{(3)})$, there corresponds a propagation direction $(-n_l^{(1)}, -n_l^{(2)}, n_l^{(3)})$. This means that the number of longitudinal normals lying outside the plane OXY has to be odd.

5 Monoclinic media: Longitudinal normals lying in the symmetry plane

The solution of the problem of longitudinal normals lying in symmetry planes is well known [9]. We discuss it here only for the reason of completeness. The plane $n_3 = 0$ will contain longitudinal normal with coordinates $[n_1, n_2, 0]$, if, and only if, equations (2a, b) are fulfilled, *i.e.* if

$$[n_l^{(1)}, n_l^{(2)}, 0] = \left[\frac{1}{c^2}\sum_{j=1}^{2}\Gamma_{1j}n_l^{(j)}, \frac{1}{c^2}\sum_{j=1}^{2}\Gamma_{2j}n_l^{(j)}, \frac{1}{c^2}\sum_{j=1}^{2}\Gamma_{3j}n_l^{(j)}\right]. \qquad (17)$$

This is equivalent to the following set of equations

$$\sum_{j=1}^{2}\Gamma_{3j}n_l^{(j)} = 0,$$
$$\left(\sum_{j=1}^{2}\Gamma_{2j}n_l^{(j)}\right)n_l^{(1)} = \left(\sum_{j=1}^{2}\Gamma_{1j}n_l^{(j)}\right)n_l^{(2)}. \qquad (18a, b)$$

For monoclinic media, equation (18a) is a trivial identity. This means that for monoclinic media one should find roots of a quartic polynomial

$$C_{26}\left(n_l^{(2)}\right)^4 + (2C_{66} - C_{22} + C_{12})\left(n_l^{(2)}\right)^3 n_l^{(1)} + (3C_{16} - 3C_{26})\left(n_l^{(2)}\right)^2\left(n_l^{(1)}\right)^2 + (C_{11} - 2C_{66} - C_{12})n_l^{(2)}\left(n_l^{(1)}\right)^3 - C_{16}\left(n_l^{(1)}\right)^4 = 0. \qquad (19)$$

Thus, the maximal number of longitudinal normals lying in the OXY plane is 4. This means that in the case of monoclinic media, in spite of the claim of Khatkevich [9], the *total* number of longitudinal normals can not be larger than 13.

6 Determination of longitudinal normals for monoclinic media

Until now we discussed the general problem of the number of longitudinal normals for monoclinic media. One may check that for monoclinic media equation (7) takes the form

$$E_{monocl}(y) = y\left(B_0 + B_2y^2 + B_4y^4 + B_6y^6 + B_8y^8\right) = 0, \qquad (20)$$

where B_0, B_2, B_4, B_6, B_8 are complicated polynomial functions of medium elastic constants of the sixth degree. We obtained their explicit form with the help of the Symbolic Computation System Maple. From equation (20), one sees that the value $y = 0$ is always the solution of equation (20). The components $n_l^{(1)}$, $n_l^{(2)}$ of the directions of the remaining longitudinal axes are determined by solving the equation

$$\left(B_0 + B_2z + B_4z^2 + B_6z^3 + B_8z^4\right) = 0, \qquad (21)$$

where $z \equiv y^2$.

The equation (21) is quartic, so it can be analytically solved, though as a rule, the appropriate analytic expressions are rather complicated. After substitution of the calculated roots into equations (15a, b), one obtains two cubic equations. Thus, generally, it is possible to obtain a closed-form expressions for directions of longitudinal normals for an arbitrary monoclinic medium.

Consider the solution $y = 0$ of equation (20). For this value of y, equations (15a, b) become

$$\left[(C_{13} - C_{33} + 2C_{55}) + (C_{11} - C_{13} - 2C_{55})\,x^2\right]x = 0,$$
$$C_{16}x^3 = 0. \qquad (22a, b)$$

The solution ($x = 0$, $y = 0$) corresponds to longitudinal normal directed along the symmetry axis. The solution $x \neq 0$ of equations (22) exists when elastic constants obey three conditions

$$C_{16} = 0,\ C_{33} = C_{11},\ C_{55} = (C_{11} - C_{13})/2. \qquad (23a\text{-}c)$$

We shall illustrate the described procedure on the example of monoclinic crystal of CDP (CsH_2PO_4), for which the matrix of elastic constants has the following form [16]:

$$\hat{C}_{CDP} = \begin{pmatrix} 28.83 & 11.4 & 42.87 & 0 & 0 & 5.13 \\ 11.4 & 26.67 & 14.5 & 0 & 0 & 8.4 \\ 42.87 & 14.5 & 65.45 & 0 & 0 & 7.5 \\ 0 & 0 & 0 & 8.1 & -2.25 & 0 \\ 0 & 0 & 0 & -2.25 & 5.2 & 0 \\ 5.13 & 8.4 & 7.5 & 0 & 0 & 9.17 \end{pmatrix}. \quad (24)$$

Units in which C_{ij} are expressed do not matter.

For the matrix $\hat{C}_{CDP}$, equation (21) could be written in the following form;

$$0.05 + 274.1z + 83.26z^2 + 135.3z^3 + 6.07z^4 = 0. \quad (25)$$

All roots of equation (25) are complex or negative. Thus, the only solution having the physical meaning is $y = 0$. This means that CDP has longitudinal normals lying in the plane OXZ. For $y = 0$ equation (15a) is a trivial identity, while equation (15b) becomes

$$(7.5 + 5.13x^2)x = 0. \quad (26)$$

The only real solution of equation (26) is $x = 0$, so the only longitudinal normal lying outside the plane OXY has components [0, 0, 1].

By solving equation (19) for the matrix of elastic constants $\hat{C}_{CDP}$, we can find longitudinal normals lying inside the plane of symmetry. The corresponding vectors $\mathbf{n}_l$ have components [0.5858, –0.8105, 0], [0.6579, 0.7531, 0]. We conclude that CDP crystal provides the example of monoclinic medium which has just 3 longitudinal normals.

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