An Attempt at Three-Dimensional Representation of Slowness Surfaces In Crystals

Garen B. Gregorian, PE, MSCE, MSME, MASCE
Project Manager,Gregorian Engineers
Email: garen@gregorianengineers.com
Zareh B. Gregorian, PE, FASCE, FACI
President,Gregorian Engineers
Email: zareh@gregorianengineers.com

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The propagation of elastic waves in crystals obeys Newton's law of motion:

$r\P^2 u_i / \P t^2 = \P s_{ij} / \P x_j$ (Eq.1)

Using the constitutive equations for a linear elastic solid relating stress and strain, to obtain an equation with only one unknown vector:

$s_{ij} = C_{ijkl} \P u_l / \P x_k$ (Eq.2)

Equation one becomes:

$r\P^2 u_i / \P t^2 = C_{ijkl} \P^2 u_l / \P x_j \P x_k$ (Eq.3)

Where C_{ijkl} is the tensor of elastic constants with 81 components. Symmetry of stress components however reduces the constants to 36 components where:

$$C_{ijkl} = C_{jikl} = C_{ijlk} = C_{jilk}$$

The existence of strain energy function further reduces the number of constants to 21.

$$C_{ijkl} = C_{klij}$$

The crystalophysical coordinate system used to measure the elastic constants is chosen along fixed crystalographic crystal axis, which reduces the number of elastic constants and simplifies the solution of the Green Christoffel equation. This coordinate system is usually set up along the symmetry axis of the crystal. The directions of the crystalophysical and crystallographic axis coincide in case of the cubic crystal.
The elastic constants of the cube with respect to a different reference frame can then be obtained by coordinate transformations of the form $A_{ij}=\alpha_{ik}\alpha_{jl}A_{kl}$.
With the Cartesian coordinate system set up along any axis, anywhere in the crystal, and if from that point a normal n called the wave normal is drawn in any direction, there are three possible phase velocities and corresponding displacement directions in which a wave could travel at that point. The phase velocities and their direction changes if the direction of the wave normal is changed. The highest phase velocity v_3, which is polarized in the direction of the wave normal, is called "Quasi-Longitudinal/Compression wave" velocity and the other two, v_1 and v_2, are called "Quasi-Transverse/Shear wave" velocities with displacement directions in a plane perpendicular to the first. Except for special directions of crystal symmetry, the quasi-longitudinal wave displacement direction is not parallel to the wave normal, but is pointed at a small angle from it. When the displacement direction is parallel to the wave normal the wave is called a "pure longitudinal wave". The axis along which transverse shear waves of equal velocity

associated with the wave normal may propagate with any wave polarization is called the acoustic axis.
The solution of equation-1 for the displacement vector of a plane wave may be put as:
$u_i(x,t) = A_i \cdot F(t-(n_1x_1+n_2x_2+n_3x_3)/\mathrm{v})$
Where A_i is the amplitude of the displacement along the i-th axis, and n_1, n_2, and n_3 are the components of the unit vector normal to the wave front.
Differentiation of $u_i(x,t)$ and substitution in left side of equation-1 gives :

$$\partial^2 u_i / \partial t^2 = A_i F''$$
$$\partial u_l / \partial x_j = -A_l n_j / \mathrm{v} \cdot F'$$
$$\partial^2 u_i / \partial x_j \partial x_k = A_l n_j n_k / \mathrm{v}^2 \cdot F''$$

Substituting in equation-3:
$$\rho A_i F'' = C_{ijkl} A_l n_j n_k$$
Introducing Acoustic tensor $\Gamma_{il} = C_{ijkl} n_j n_k$ in equation-3 and simplifying, yields:
$$\left| \Gamma_{il} - \rho \mathrm{v}^2 \delta_{il} \right| = 0 \quad \text{(Eq.4)}$$
Equation-4 is referred to as Christoffel's Equation or the Secular Equation and solution of the determinant provides us with a cubic equation, the roots of which are the eigenvalues of the Γ_{il} tensor. The eigenvalues of the Γ_{il} tensor are the phase velocities of the wave propagating in the medium in a given direction. The eigenvectors of the Γ_{il} tensor give us the directions of the displacement vector for the corresponding phase velocities of the waves propagating in the crystal.
The Γ_{il} tensor has in general three distinct eigenvalues (phase velocities) and eigenvectors (displacement directions) in any given direction of the wave normal n. The three eigenvalues have in general different values, except for special directions of symmetry. The slowness surfaces have three sheets with the slowness surface corresponding to the quasi-longitudinal wave with the highest phase velocity contained in the other two surfaces. This means that a line drawn parallel to the wave normal from the origin will in general intersect the surfaces three times. For crystals of most materials in certain directions, the slowness surfaces do in fact cross one another or become tangent. In the crystal of Gallium Arsenide for example, the three slowness surfaces do not cross one another along the face of the cube but become tangent along the acoustic axis. Cross section of the plane of the diagonal of the cube shows that the pure shear wave crosses the quasi shear wave along the three-fold axis of symmetry of the cube.
The magnitude and direction of waves propagating in an elastic solid has been modeled with a worksheet developed within Mathcad computer software program to use the elastic constants of the material to setup the Γ_{il} tensor of equation 4 and solve for the determinant on the left side. Solution of the determinant incorporates solving a cubic equation with coefficients of the Γ_{il} tensor which are made up of the direction cosines of the wave normal coupled with the elastic constants in the form, $\Gamma_{il} = C_{ijkl} n_j n_k$. The wave normal, in general, has direction cosines $n_1=\sin\theta\cos\alpha$, $n_2=\sin\theta\sin\alpha$ and $n_3=\cos\theta$, where α is the angle between the projection of the wave normal on the x-y plane and the x axis, and θ, is the angle between the wave normal and the z axis called the polar angle, as in spherical coordinate system. As an example, the Γ_{11} term would look like:
$$\Gamma_{11} = c_{11}n_1^2 + c_{66}n_2^2 + c_{55}n_3^2 + 2c_{16}n_1n_2 + 2c_{15}n_1n_3 + 2c_{56}n_2n_3$$

The roots of the cubic equation found by an algebraic subroutine displays the roots in the customary form with decreasing orders of magnitude. This means that $v_3>v_2>v_1$ for every direction of the wave normal where the eigenvalues are distinct. In crystal of Gallium Arsenide(GaAs), $\bar{4}3m$, with the wave normal parallel to the xy plane, the three surfaces do not cross one another. They become tangent along the acoustic axis.(Figure-1) For special directions of the wave normal, however, the cubic equation factors into a linear term and a quadratic term analytically and gives us the value of one of the velocities directly. This velocity is greater than the other velocities in some directions and is smaller than them in other directions as can be seen in figure-3.

With the wave normal along the cube diagonal, however, the Pure shear wave v_2 is greater than pure Quasi shear wave v_1 for θ of about 0 degrees to about 45 degrees, and is smaller than v_1 for θ between 45 and 90 degrees. In other words, the two surfaces v_2 and v_1 do in fact cross one another. This result is obvious if the velocities are solved for analytically. If the eigenvalues are solved for numerically however, then v_2 is always greater than v_1, and the two surfaces never cross one another. To plot the slowness surfaces using the computer program, the velocities were solved for directly by solving for the larger root and plugging back into the cubic equation to solve for the remaining quadratic equation after it's extraction. In this case, v_2 was always greater than v_1 the two surfaces did not cross one another. The plot of the incorrect and correct velocity surfaces are shown in Figures 2 and 3, respectively. An extensive computation of the slowness surfaces of crystals of cubic symmetry was carried out by Miller and Musgrave in 1956. Wire models were used to help describe the various irreducible portions of the wave surfaces.

Directions of wave propagation where the acoustic tensor is simplified by analytical methods is illustrated by the following example.

Gallium Arsenide(GaAs, Cubic), $\bar{4}3m$, has the following elastic constants:
$c_{11}=11.88\text{x}10^{10}$, $c_{12}=5.38\text{x}10^{10}$, $c_{44}=5.94\text{x}10^{10}$ [Newtons/m^2].

If the propagation vector is directed parallel to X-Y plane on the cube face, the secular equation can be factored and solved analytically. With the wave normals $n_1=\cos\alpha$, $n_2=\sin\alpha$ and $n_3=0$, the Γ_{il} tensor takes the form:

$$\Gamma_{il} = \begin{vmatrix} \Gamma_{11} & \Gamma_{12} & 0 \\ \Gamma_{12} & \Gamma_{22} & 0 \\ 0 & 0 & \Gamma_{33} \end{vmatrix}$$

With components:

$$\Gamma_{11} = c_{11}\cos^2 a + c_{44}\sin^2 a \qquad \Gamma_{12} = (c_{12} + c_{44})\cdot \sin 2a / 2$$

$$\Gamma_{22} = c_{11}\sin^2 a + c_{44}\cos^2 a \qquad \Gamma_{33} = c_{44}\cos^2 a + c_{44}\sin^2 a$$

Substituting in the determinant and solving for the velocities we obtain:

$$v_1 = \sqrt{\Gamma_{33}/r} = \sqrt{c_{44}\cos^2 a + c_{44}\sin^2 a / r}$$

$$v^2{}_{2,3} = \frac{\Gamma 11 + \Gamma 22 \pm \sqrt{(\Gamma 11 - \Gamma 22)^2 + 4\Gamma 12^2}}{2 \cdot r}$$

Note that the solution v_1 is the factored linear term directly obtained to be

$v_1 = \sqrt{\Gamma_{33}/r} = \sqrt{c_{44}/r}$ which is a pure shear wave shown in Figure-1.

The quasi-longitudinal and quasi shear waves are obtained by solving the quadratic part. Note that in this cross section the slowness surfaces do not cross one another but have the same magnitude along the acoustic axis, along the fourfold crystal axis. This solution and surface plot can easily be obtained by the computer worksheet since the surfaces do not cross one another in all the directions of the polar angle α. Proper interpretation of the results is a must however and one should not rely solely on the computer program.

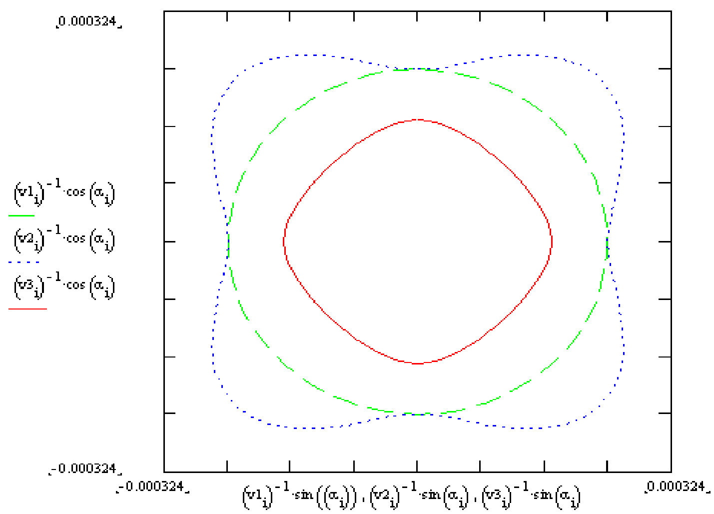


Figure 1. Slowness surface for GaAs Wave normal Parallel to xy plane
Crossection of xy plane

Next we direct the propagation vector along the diagonal plane of the cube. The secular equation can be factored and solved analytically after performing the proper coordinate transformations on the stiffness matrix. With the wave normals n_1=sinθ, n_2=0 and n_3=cosθ, and α=45 degrees, the Γ_{il} tensor takes the form:

$$\Gamma'_{il} = \begin{vmatrix} \Gamma'_{11} & 0 & \Gamma'_{13} \\ 0 & \Gamma'_{22} & 0 \\ \Gamma'_{13} & 0 & \Gamma'_{33} \end{vmatrix}$$

With components:

$$\Gamma'_{11} = c'_{11}\sin^2 q + c'_{44}\cos^2 q \qquad \Gamma'_{13} = (c'_{13} + c'_{44}/2)\cdot \sin 2q$$

$$\Gamma'_{22} = c'_{66}\sin^2 q + c'_{44}\cos^2 q \qquad \Gamma'_{33} = c'_{44}\sin^2 q + c'_{33}\cos^2 q$$

Where c'_{11}, c'_{22}, etc., are the stiffness constants of the crystal in the rotated reference frame, obtained by coordinate transformation. In this case 45 degrees about the z axis and 45 degrees about the transformed y axis. Substituting in the determinant and solving for the eigenvalues we obtain:

$$v_2 = \sqrt{\Gamma'_{22}/r} = \sqrt{c'_{66}\sin^2 q + c'_{44}\cos^2 q / r}$$

$$v^2_{3,1} = \frac{\Gamma'11 + \Gamma'33 \pm \sqrt{(\Gamma'11 - \Gamma'33)^2 + 4\Gamma'13^2}}{2\cdot r}$$

The pure shear wave v_2 with the displacement direction parallel to the X-Z plane is obtained readily as a linear factor multiplied by a quadratic term to make up the cubic equation, which results from solving for the determinant of the Γ_{il} tensor.(Figure-3) Graph of the Slowness surfaces obtained by the computer program, however, shows the three surface contained within one another as $v_3>v_2>v_1$ in all directions.(Figure-2)

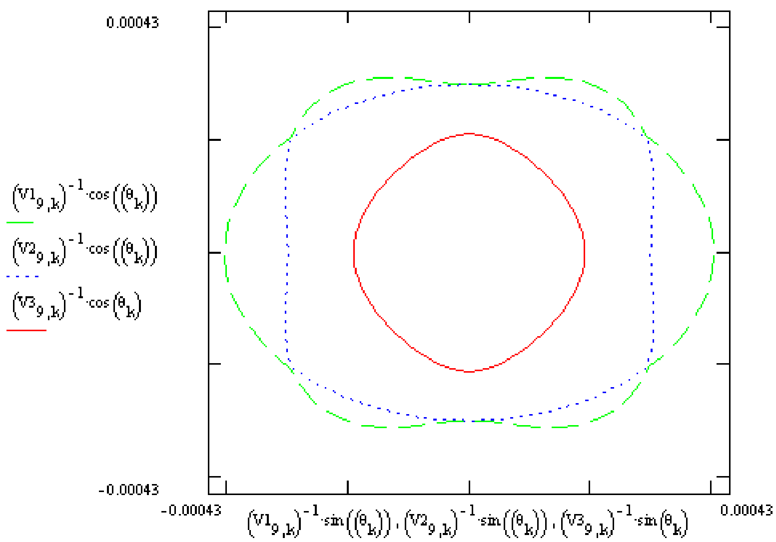


Figure 2. Slowness surface for GaAs,Wave normal along cube diagonal
Plot of Computer Program

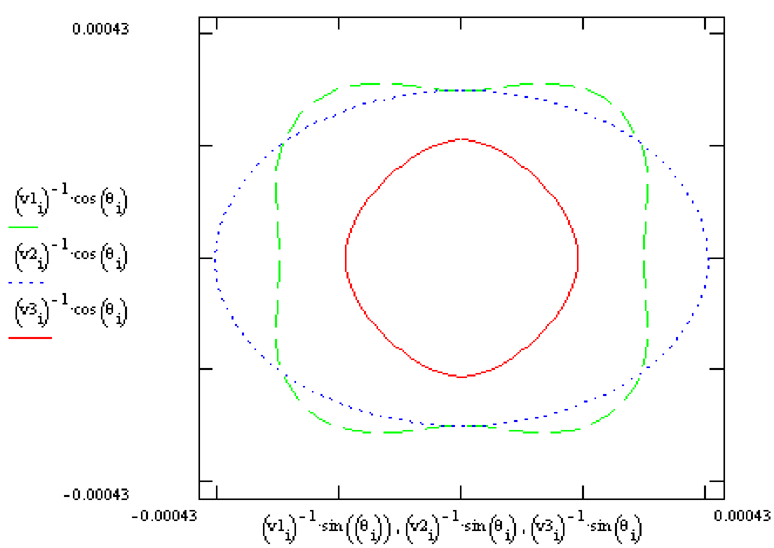


Figure-3 Slowness Surface for GaAs, Wave normal along cube diagonal
Plot of Analytical Solution

For a second example we look at the crystal of Tellurium dioxide. Tellurium dioxide (Tetragonal 422) has the following elastic constants: $c_{11}=5.57\text{x}10^{10}$, $c_{12}=5.12\text{x}10^{10}$, $c_{13}=2.18\text{x}10^{10}$, $c_{33}=10.58\text{x}10^{10}$, $c_{44}=2.65\text{x}10^{10}$, $c_{66}=6.59\text{x}10^{10}$ [Newtons/m^2]. If the propagation vector is directed parallel to the X-Z plane, the secular equation can be factored and solved analytically. With the wave normals $n_1=\sin\theta$, $n_2=0$ and $n_3=\cos\theta$, and $\alpha=0$ degrees, the Γ_{il} tensor takes the form:

$$\Gamma_{il} = \begin{vmatrix} \Gamma_{11} & 0 & \Gamma_{13} \\ 0 & \Gamma_{22} & 0 \\ \Gamma_{13} & 0 & \Gamma_{33} \end{vmatrix}$$

With components:

$$\Gamma_{11} = c_{11}\sin^2 q + c_{55}\cos^2 q \qquad \Gamma_{13} = (c_{13}+c_{55})/2\cdot\sin 2q$$

$$\Gamma_{22} = c_{66}\sin^2 q + c_{55}\cos^2 q \qquad \Gamma_{33} = c_{55}\sin^2 q + c_{33}\cos^2 q$$

Solving for the eigenvalues of the Γil matrix:

$$\begin{vmatrix} (\Gamma_{11}-l) & 0 & \Gamma_{13} \\ 0 & (\Gamma_{22}-l) & 0 \\ \Gamma_{13} & 0 & (\Gamma_{33}-l) \end{vmatrix} = (\Gamma_{22}-l)[(\Gamma_{11}-l)\cdot(\Gamma_{33}-l)-\Gamma_{13}^2]$$

Where the pure shear wave is readily obtained from the linear term, $(\Gamma_{22}-\lambda)=0$ as:

$$v_2 = \sqrt{\Gamma_{22}/r} = \sqrt{c_{66}\sin^2 q + c_{44}\cos^2 q / r}$$

The longitudinal and transverse shear waves are obtained by solving the quadratic term as:

$$V^2_{1,3} = \frac{\Gamma 11 + \Gamma 33 \pm \sqrt{(\Gamma 11 - \Gamma 33)^2 + 4\Gamma 13^2}}{2\cdot r}$$

As we can see in the compliance tensor $c_{66}>c_{11}$, and c_{44} is as usual smaller than c_{11} . If we plot the slowness curves for the crossection on the face of the cube x-z, we can see that the curve for the longitudinal wave v_3 crosses the curve v_2 for the pure shear wave along the x axis. This can be seen in figure-4.

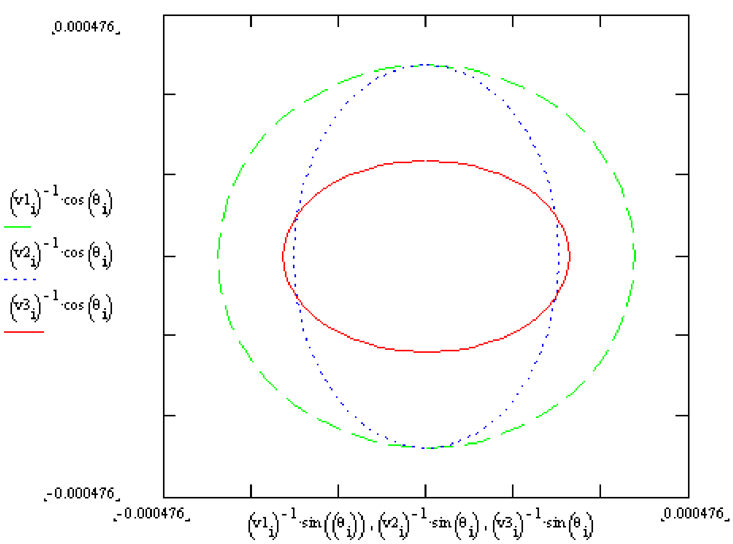


Figure-4. Propagation of waves in TeO2. Wave normal parallel to X-Z plane. Plot of Analytical Solution

The same crossection is plotted by the Mathcad worksheet, which calculates the eigenvalues by numerically solving the cubic equation. The velocity surfaces v_2 and v_3 do not cross one another in this case.(Figure-5)

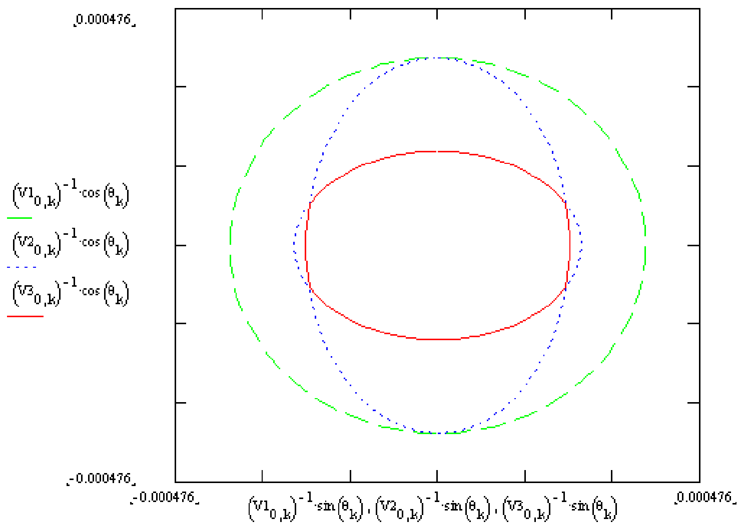


Figure-5. Slowness Surface for TeO2, Wave normal parallel to X-Z plane. Plot of Computer Solution

Conclusion:

The equation of propagation of acoustic waves in crystals was derived from Newton's second law and solved for using conventional methods of tensor calculus and linear algebra. Propagation of elastic waves was investigated for crystals of cubic and tetragonal classes by generating slowness surfaces for various directions of crystal symmetry. The characteristic equation, which results from attempting to solve of the Green Christoffel equation, is a third degree polynomial which can not be solved directly to obtain the eigenvalues. General methods of solution to the cubic equation are not suitable for numerical computation and do not provide the correct inverse velocity surfaces. Analytical solution may be used for special directions of crystal symmetry where the third degree polynomial can be factored to a linear and a quadratic term but for other directions, wire models have been known to help describe the correct surface.

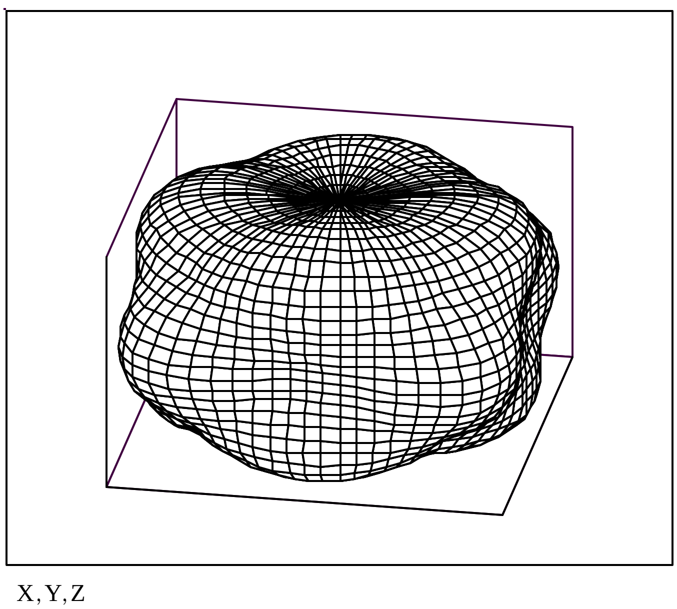
References:

1. Fedor I. Fedorov, *Theory of Elastic Waves in Crystals*, Plenum Press, New York, 1968.
2. M.J.P. Musgrave, *Crystal Acoustics*, Holden-Day, Inc., San Francisco, CA, 1970.
3. G.F. Miller and M.J.P. Musgrave, On The Propagation of Elastic Waves in Aelotropic Media. III Media of Cubic Symmetry., Proceedings of Royal Society, A, 236, 352(1956).
4. J. F. Nye, *Physical Properties of Crystals*, Oxford University Press, 1957.
5. E. Dieluesaint and D. Royer, *Elastic Waves in Solids, Applications to Signal Processing*, John Wiley & Sons, New York, 1980.

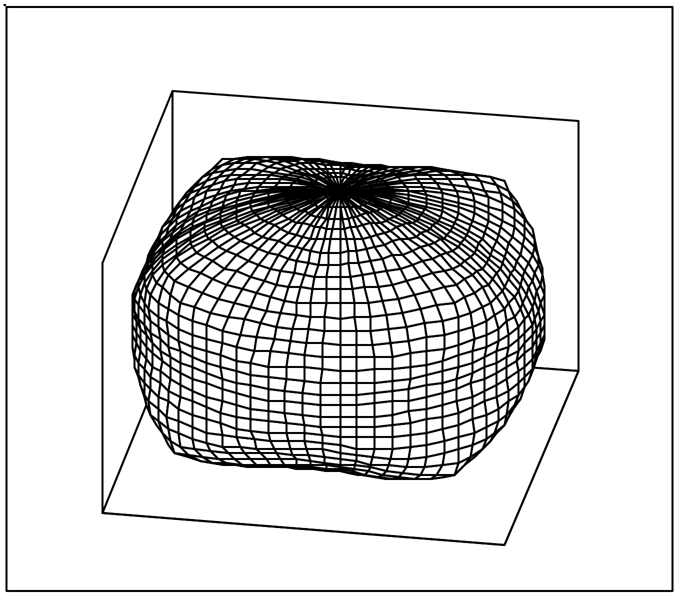
6. B. A. Auld, *Acoustic Fields and Waves in Solids*, John Wiley & Sons, New York, 1973.
7. A. E. H. Love, *A Treatise On The Mathematical Theory of Elasticity*, Dover Publications, New York, 1944.
8. I. S. Sokolnikoff, *Mathematical theory of Elasticity*, McGraw-Hill New York, 1946.
9. S. Timoshenko and J. Goodier, *Theory of Elasticity*, McGraw-Hill, New York, 1970.
10. J. V. Uspenski, *Theory of Equations*, McGraw-Hill, New York, 1948.
11. J. J. Tuma, *Engineering Mathematics Handbook*, Third Edition, McGraw-Hill, New York, 1987.
12. Mathcad Professional Users Guide, MathSoft, Inc., Cambridge, MA, 1997.

Appendix:

Three-dimensional graphs of the slowness surfaces generated by the computer worksheet (which does not incorporate intersection of surfaces for v_1 and v_2) for v_1, v_2 and v_3 of Gallium Arsenide are incorporated for information purposes.

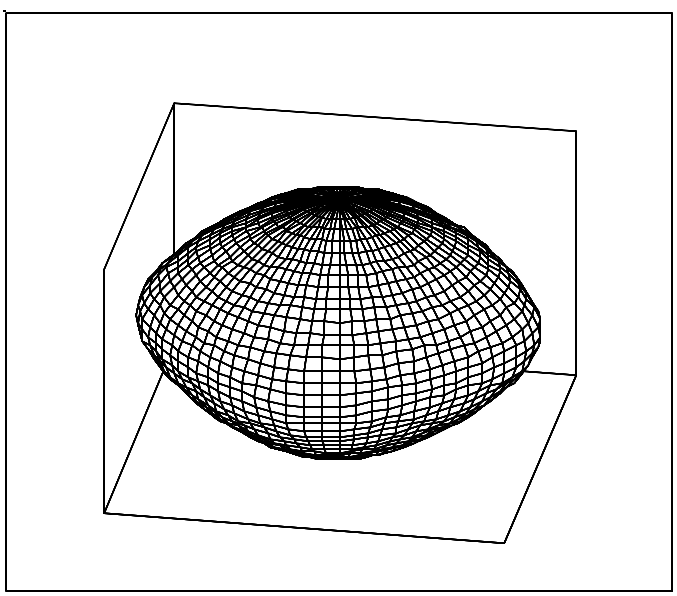


Slowness Surface $1/v_1$ For Gallium Arsenide
Worksheet Solution



X, Y, Z

Slowness Surface $1/v_2$ For Gallium Arsenide
Worksheet Solution



X, Y, Z

Slowness Surface $1/v_3$ For Gallium Arsenide
Worksheet Solution