OLVING SNELL'S LAW

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Introduction

A wave obliquely impinging on the boundary between two different materials generates reflected and refracted waves. Calculation of such emergent waves is usually performed in two steps [1.2]. First, Snell's law is used for determining the speed and the propagation infection of the emergent waves. Second, the emergent amplitudes are evaluated by imposing the relevant boundary conditions. The peculiar difference between the two steps is that the former is a general consequence of the geometric properties of the interaction whereas the latter accounts for the dynamic aspects of the specific problem.

From a mathematical point of view this procedure exhibits unsuspected drawback: and pitfalls due mainly to several algebraic difficulties. Precisely, the determination of the amplitudes always results in solving a linear algebraic system; notwithstanding this, the rank of such a system can hardly be determined at a very general level and, what is more such a rank can depend on the value of the angle of incidence (see [3] for the case of linea crystals). On the other hand, also for linear wave propagation Snell's law leads usuall o nonlinear equations; consequently, even determining the number of the emergent waves seems to be a formidable task.

In this note we present a physical example exhibiting all the prominent mathematical features which are encountered when solving Snell's law. Specifically, we determine the admissible refracted waves propagating in rutile (TiO₂), a tetragonal crystal belonging to class 4/mmm: the explicit calculation of both the propagation speeds and the angles of refraction in terms of the angle of incidence allows us to point out some not obvious aspects concerning Snell's law.

A peculiar result is obtained in conjunction with evanescent waves, namely waves whose amplitude vanishes exponentially at infinity. We show that evanescent waves can be generated whose propagation speed takes on complex value. Unlike standard evanescent waves having a complex angle of refraction but a real speed of propagation, we explicitly prove that waves traveling at a complex speed are compatible with a flow of energy across the boundary.

Elastic waves

The propagation speeds V of plane (exponential) waves traveling along a direction n_r in a hyperelastic crystal with a stiffness tensor c_{prsq} and mass density ρ are the roots of the secular equation [1,4]

$$|\Gamma_{pq} - \rho V^2 \delta_{pq}| = 0, \qquad (1)$$

where the acoustic tensor

$$\Gamma_{pq} = c_{prsq} n_r n_s$$

is a symmetric and positive definite tensor. We assume that, for any real frequency ω , the elastic displacement is given by the real part of the quantity

$$u_r = \mathcal{U}\Pi_r \exp\left\{i\omega\left(t - \frac{n_r x_r}{V}\right)\right\}, \qquad i = \sqrt{-1},$$
(2)

where the polarization vector Π_r is an eigenvector of the acoustic tensor Γ_{pq} associated with the eigenvalue ρV^2 , whereas the amplitude \mathcal{U} is determined by suitable boundary or initial conditions.

Consider wave propagation in crystals belonging to the tetragonal system and suppose that the propagation takes place in the plane (001) perpendicular to the tetrad axis Choose the x and y axes as the [100] and [010] directions respectively, and let $(\mu, \sigma, 0)$ be the components of the unit vector n_r , so that $\mu^2 + \sigma^2 = 1$. Then the nonvanishing I's are given by [4, p. 190]

$$\begin{split} \Gamma_{11} &= c_{1111} \mu^2 + c_{1212} \sigma^2 + 2 c_{1112} \mu \sigma, \qquad \Gamma_{12} &= c_{1112} (\mu^2 - \sigma^2) + (c_{1122} + c_{1212}) \mu \sigma \\ \Gamma_{22} &= c_{1212} \mu^2 + c_{1111} \sigma^2 - 2 c_{1112} \mu \sigma, \qquad \Gamma_{33} &= c_{2323}. \end{split}$$

In the case of rutile we have the following experimental data [5]

$$c_{1111} = 27.3 \cdot 10^{10} \frac{\text{N}}{\text{m}^2}, \qquad c_{1122} = 17.6 \cdot 10^{10} \frac{\text{N}}{\text{m}^2},$$
$$c_{1212} = 19.4 \cdot 10^{10} \frac{\text{N}}{\text{m}^2}, \qquad c_{2323} = 12.5 \cdot 10^{10} \frac{\text{N}}{\text{m}^2},$$

$$\rho = 4.25 \cdot 10^3 \frac{\mathrm{kg}}{\mathrm{m}^3},$$

long with the exact condition $c_{1112} = 0$. Accordingly, the roots of the secular equation 1) are

$$2\rho V_{\pm}^2 = W_{\pm}^2(\mu) \cdot 10^{10},\tag{3}$$

$$\rho V_3^2 = \Gamma_{33} = 12.5 \cdot 10^{10}, \tag{4}$$

vhere

$$W_{\pm}^{2}(\mu) = 46.7 \pm \sqrt{62.41 + 5226.36(\mu^{2} - \mu^{4})};$$
(5)

is usual, the three propagation speeds are defined to be the positive roots of (3) and (4). The polarization vectors relative to the previous speeds are easily calculated. We have

$$\Pi_r^{\pm} = \begin{pmatrix} -37.0\mu\sigma\\ 19.4 + 7.9\mu^2 - \frac{1}{2}W_{\pm}^2\\ 0 \end{pmatrix}$$
(6)

$$\Pi_r^3 = \begin{pmatrix} 0\\0\\1 \end{pmatrix} \tag{7}$$

In agreement with the current terminology, the speed V_3 corresponds to a shear wave polarized along the direction [001], while V_- and V_+ are the propagation speeds of ε quasishear and a quasilongitudinal wave, respectively, whose polarization vectors belong to the plane (001).

Snell's law

Suppose now that rutile occupies the upper half space y > 0 whereas in the lower hal space is present an elastic crystal where the slowest speed is lower than the slowest speed in rutile. Suppose also that an incident wave, traveling at speed $V_{\rm inc}$ along the direction $(\mu_{\rm inc}, \sigma_{\rm inc}, 0), \ \mu_{\rm inc} > 0, \ \sigma_{\rm inc} > 0$, collides with the boundary so that the refracted waves in rutile propagate and are polarized in the plane (001) as described in the previous section According to Snell's law [2,4], the quantity V/μ takes the same value for every wave namely

$$\left(\frac{V}{\mu}\right)_{\text{emergent}} = \frac{V_{\text{inc}}}{\mu_{\text{inc}}}.$$
(8)

Since the refracted waves are polarized in the plane (001), we get the first result that no waves traveling at speed V_3 are generated. Accordingly, look at the two wave propagating at speed V_{\pm} . In terms of the quantity α defined by the relationship

$$\frac{V_{\rm inc}}{\mu_{\rm inc}} = \frac{10^5}{\sqrt{2\rho}} \, \alpha \approx 1084.65 \alpha, \qquad \alpha > 0, \tag{9}$$

Snell's law (8) can be written as

$$\alpha = \frac{W_+}{\mu_+} = \frac{W_-}{\mu_-}.$$
 (10)

Substitution of (10) into (5) gives rise to an equation for μ_+ and to an equation for μ_- both of which can be solved by isolating the radical terms and squaring. In so doing the same equation for μ_+ and μ_- is arrived at; consistently, the subscripts \pm will be omitted The resulting equation is

$$(5226.36 + \alpha^4)\mu^4 - (5226.36 + 93.4\alpha^2)\mu^2 + 2118.48 = 0.$$
(11)

Solutions to (11) provide the possible values of the quantity μ . The admissible μ 's, along with the corresponding speeds, are to be found from (10) with the only constraint that n view of (9), the ratio W/μ must be positive. For further reference, we point out that condition (10) implies also that the quantities $W_{\pm}(\mu)$ take on complex values if and only f μ becomes a complex quantity.

Determination of μ

It is a consequence of (11) that every solution μ depends on the value of α , a quantity which is ultimately determined by the angle of incidence. A qualitative discussion about the behavior of the function $\mu = \mu(\alpha)$ can be done with the aid of the graphic method for solving Snell's law—see, e.g., [4, p. 203]—which relies on the use of the so-called slownes surfaces, namely the locus of the tips of the vectors n_r/V . However, it should be noticed in advance that this method provides only those real values of μ satisfying the condition $\mu \leq 1$. The other values single out the evanescent waves, which must be considered in order that the amplitudes of all emergent waves can uniquely be determined—a discussion on this point is presented in [6].

In the case at hand, the slowness curves of rutile, i.e. the cross section of the slowness surfaces of rutile relative to the speeds W_{\pm} by plane (001), are shown in fig. 1, where four points are marked by a tick. The explicit values of the quantity α corresponding to them are easily calculated. The value α_{+} is determined by the intersection of the slowness curve W_{+} with the horizontal—or vertical—axis; accordingly it turns out that

$$\alpha_+ = W_+(1) = W_+(0) \approx 7.39.$$

Similarly, the value α_{-} corresponds to the intersection of the slowness curve W_{-} with the horizontal axis; hence

$$\alpha_{-} = W_{-}(1) = W_{-}(0) \approx 6.23.$$



Fig. 1 Slowness curves for rutile

The value α_0 is determined in the following way. Let μ_0 be such that $W_+(\mu_0) = W_-(\mu_0) = 16.7$. In view of (5) we obtain $\mu_0 \approx 1.012$. Then condition (10) implies that

$$\alpha_0 \approx 6.79$$

Ne remark that, for $\alpha = \alpha_0$, the two polarization vectors (6) coincide.

Finally, the value of α_c is the real value of α for which the discriminant of (11) vanishes. Ne get

 $\alpha_c \approx 4.16.$

It is worthwhile to notice that α_c plays the role of a critical threshold in that, for $\alpha < \alpha_c$, the quantity μ takes on complex values.

The relevance of the previous points is that they define five intervals, determining the qualitative behavior of the solution μ to (11) as follows.

- $\alpha_+ \leq \alpha$: there are two distinct real values of μ lower than 1; as fig. 1 shows, one speed belongs to the slowness curve W_+ and the other to the slowness curve W_- .
- $\alpha_0 < \alpha < \alpha_+$: there are two real solutions for μ , but only one is lower than 1. For $\mu < 1$ the speed belongs to the slowness curve W_- whereas for $\mu > 1$ the speed can be calculated by means of the function $W_+(\mu)$.
 - $\alpha = \alpha_0$: as before, but for $\mu_0 = \mu(\alpha_0) > 1$ we have $W_+(\mu_0) = W_-(\mu_0)$.
- $\alpha_{-} < \alpha < \alpha_{0}$: as before, but from now on both speeds must be determined through the function $W_{-}(\mu)$.
- $\alpha_c < \alpha \leq \alpha_-$: there are again two distinct real values of μ lower than 1, both speeds belonging to the slowness curve W_- .

 $\alpha = \alpha_c$: the two real values of μ lower than 1 now coincides.

 $\alpha < \alpha_c$: the quantity μ becomes a complex number.

Note that, for $\alpha = \alpha_c$, the slowest speed V_{slow} in rutile is reached; precisely we have $V_{\text{slow}} \approx 3550 \text{ m/s}$.

Evanescent waves

As is well known, evanescent waves occur typically when μ takes on real values greate: than 1. Here, however, we have exhibited a physical example in which μ is allowed to become even a complex number; in turn, this implies that also the corresponding speed Vpossesses a nonvanishing imaginary part. This last section is devoted to investigate such a circumstance.

The first problem that arises is how to choose two appropriate solutions out of the four ones relative to (11). Indeed this is a matter of convention; on denoting the real par of a complex quantity ξ by the symbol $\Re(\xi)$, we stipulate that $\Re(\mu) > 0$ so as to retain the continuity of the function $\mu(\alpha)$.

To fix notation, we set

$$\mu = \mu_{(1)} + i\mu_{(2)}, \qquad \sigma = \sigma_{(1)} + i\sigma_{(2)}, \qquad V = V_{(1)} + iV_{(2)}.$$
 (12)

Since α is a real and positive quantity, Snell's law (8) and condition (9) give

$$V_{(1)} + iV_{(2)} = 1084.65\alpha(\mu_{(1)} + i\mu_{(2)}) \iff 1084.65\alpha = \frac{V_{(1)}}{\mu_{(1)}} = \frac{V_{(2)}}{\mu_{(2)}},$$
 (13)

whereby condition $\mu_{(1)} > 0$ implies $V_{(1)} > 0$.

Look now at the quantity (2); on using relation (13), ultimately we get

$$u_{r} = \mathcal{U}\Pi_{r} \exp\left\{\omega \frac{\mu_{(1)}}{V_{(1)}} \frac{\mu_{(1)}\sigma_{(2)} - \mu_{(2)}\sigma_{(1)}}{\mu_{(1)}^{2} + \mu_{(2)}^{2}} y\right\} \times \exp\left\{i\omega\left(t - \frac{\mu_{(1)}}{V_{(1)}} x - \frac{\mu_{(1)}}{V_{(1)}} \frac{\mu_{(1)}\sigma_{(1)} + \mu_{(2)}\sigma_{(2)}}{\mu_{(1)}^{2} + \mu_{(2)}^{2}} y\right)\right\}.$$
 (14)

The appearance of the complex quantities (12) is completely justified by (14) which shows that the function $\Re(u_r)$ represents a wave traveling at speed

$$V_{\text{phase}} = V_{(1)} \frac{(\mu_{(1)}^2 + \mu_{(2)}^2)/\mu_{(1)}}{\sqrt{(\mu_{(1)}^2 + \mu_{(2)}^2)^2 + (\mu_{(1)}\sigma_{(1)} + \mu_{(2)}\sigma_{(2)})^2}}$$

along the (real) direction

$$n_r = \frac{(\mu_{(1)}^2 + \mu_{(2)}^2)\delta_{1r} + (\mu_{(1)}\sigma_{(1)} + \mu_{(2)}\sigma_{(2)})\delta_{2r}}{\sqrt{(\mu_{(1)}^2 + \mu_{(2)}^2)^2 + (\mu_{(1)}\sigma_{(1)} + \mu_{(2)}\sigma_{(2)})^2}};$$

the amplitude of this wave decrease to zero as $y \to \infty$ provided that $\mu_{(2)}$ and $\sigma_{(2)}$ do not vanish simultaneously, thus ruling out the case $\mu \leq 1$. Of course, the vanishing of the amplitude at infinity requires that

$$\mu_{(1)}\sigma_{(2)} - \mu_{(2)}\sigma_{(1)} < 0;$$

in view of $\sigma^2 = 1 - \mu^2$, this condition is tantamount to choosing $\sigma_{(2)} < 0$.

We are now interested in determining whether there is an average flow of energy across the boundary in conjunction with the wave (14). Such a flow can be calculated as the integral of the time average of the elastic Poynting vector

$$P_r = -T_{sr} \frac{\partial u_s}{\partial t} = -c_{rspq} \frac{\partial u_p}{\partial x_q} \frac{\partial u_s}{\partial t}$$
(15)

over the boundary [4, p. 173]. Therefore, it suffices that we evaluate the time average of the quantity (15). On denoting time average by angle brackets, it is easy to prove that for arbitrary time harmonic functions $f \exp(i\omega t)$ and $g \exp(i\omega t)$, [7, p. 57]

$$\langle \Re[f \exp(i\omega t)] \,\Re[g \exp(i\omega t)] \rangle = \frac{\omega}{2\pi} \,\int_0^{2\pi/\omega} \Re[f \exp(i\omega t)] \,\Re[g \exp(i\omega t)] \,dt = \frac{1}{2} \Re(fg^*), \quad (16)$$

star denoting the complex conjugate. Since the unit normal to the boundary is $N_r = \delta_{r2}$ n view of (14)-(16) we arrive at the formula

$$\langle P_{r}N_{r}\rangle = \langle P_{2}\rangle = \frac{1}{2}\omega^{2}|\mathcal{U}|^{2} \exp\left\{ 2\omega \frac{\mu_{(1)}}{V_{(1)}} \frac{\mu_{(1)}\sigma_{(2)} - \mu_{(2)}\sigma_{(1)}}{\mu_{(1)}^{2} + \mu_{(2)}^{2}} y \right\} \times \\ \frac{\mu_{(1)}}{V_{(1)}} \left[c_{s2p1} \Re(\Pi_{s}^{*}\Pi_{p}) + \frac{\mu_{(1)}\sigma_{(1)} + \mu_{(2)}\sigma_{(2)}}{\mu_{(1)}^{2} + \mu_{(2)}^{2}} c_{s2p2} \Re(\Pi_{s}^{*}\Pi_{p}) + \frac{\mu_{(1)}\sigma_{(2)} - \mu_{(2)}\sigma_{(1)}}{\mu_{(1)}^{2} + \mu_{(2)}^{2}} c_{s2p2} \Re(i\Pi_{s}^{*}\Pi_{p}) \right].$$
(17)

A more convenient form for the formula (17) can be gained as follows. As the acoustic ensor is positive definite, we have

$$c_{s2p2}\Pi_s^*\Pi_p = (c_{srpq}N_rN_q)\Pi_s^*\Pi_p = \Gamma_{sp}\Pi_s^*\Pi_p \in \mathbb{R}.$$

Also, on letting $\Pi_r = \Phi_r + i\Psi_r$, we find that

$$c_{s2p1}\Re(\Pi_s^*\Pi_p) = (c_{1122} + c_{1212})(\Phi_1\Phi_2 + \Psi_1\Psi_2).$$

Accordingly, (17) reduces to

$$\langle P_2 \rangle = \frac{1}{2} \omega^2 |\mathcal{U}|^2 \exp \left\{ 2\omega \frac{\mu_{(1)}}{V_{(1)}} \frac{\mu_{(1)}\sigma_{(2)} - \mu_{(2)}\sigma_{(1)}}{\mu_{(1)}^2 + \mu_{(2)}^2} y \right\} \times$$

$$\frac{\mu_{(1)}}{V_{(1)}} \left[(c_{1122} + c_{1212})(\Phi_1 \Phi_2 + \Psi_1 \Psi_2) + \frac{\mu_{(1)}\sigma_{(1)} + \mu_{(2)}\sigma_{(2)}}{\mu_{(1)}^2 + \mu_{(2)}^2} c_{s2p2} \Pi_s^* \Pi_p \right].$$
(18)

We are now in a position to discuss the three cases $\mu \leq 1, \mu > 1$, and μ complex. In the first case $\mu_{(2)} = 0$, $\sigma_{(2)} = 0$, and $\Psi_r = 0$. Therefore in accordance with (18) we have $\langle P_2 \rangle \neq 0$, i.e. energy flows across the boundary. On the other hand, when $\mu > 1$ we have $u_{(2)} = 0$ and $\sigma = i\sigma_{(2)}$. In this instance it follows from (6) that Φ_r is proportional to δ_{2r} and that $\Psi_r = -37.0\mu\sigma_{(2)}\delta_{1r}$. Collecting these results we find that $\langle P_2 \rangle = 0$, namely for a standard evanescent wave there is no flow of energy across the boundary.

Finally, consider an evanescent wave where μ takes on a complex value. It follows from (18) that $\langle P_2 \rangle \neq 0$; in other word, energy is allowed to flow across the boundary. As a result, evanescent waves with a complex μ are compatible with a flow of energy across the boundary, whereas standard evanescent waves are not.

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