

Interpretation of Torsional Frequencies of Crystal Specimens

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(Received September 12, 1940)

A crystalline cylinder when subjected to a harmonically varying twisting moment in general not only twists but bends. A correct interpretation of the response frequencies is important in dynamical determinations of the elastic constants of crystals, and it is desirable that the measurements be made under such conditions that a simple formula, similar to that for isotropic materials, may be used without fear of serious error. In static measurements two such formulas are required, one for twist with bending prevented and the other for twist with bending unrestrained. It is shown here that each of these is a good approximation in dynamic measurements over certain

ranges of frequencies and of specimen lengths, and formulas are derived by which the errors may be estimated. A simple straight-line plot based on approximate values of the elastic constants gives all the information that is needed for the selection of good working conditions in the final measurements. For the sodium and copper-gold crystals on which measurements have been reported, the pure torsion formula is a good approximation when no parasitic response frequencies are observable; but it would cease to be a good approximation for specimen lengths below about 3 cm.

IN a crystalline cylinder whose axis is oriented arbitrarily with respect to the crystal axes, application of either a bending or a twisting moment alone produces both bending and twisting. In static experiments the effective Young's modulus E' and rigidity G' measured under these conditions differ from the values E and G obtained when only pure bending or pure twist is allowed to occur.¹ If the specimen axis is Oz and if the plane of the torsion-coupled bending is taken as the zx plane, then in terms of the elastic moduli s_{ij}' referred to the xyz axes

$$\begin{aligned} E' &= E(1 - \epsilon) = 1/s_{33}', \\ G' &= G(1 - \epsilon) = 2/(s_{44}' + s_{55}'), \\ \epsilon &= s_{34}'^2/s_{33}'(s_{44}' + s_{55}'). \end{aligned} \quad (1)$$

In dynamic measurements of the elastic constants of crystals, it has usually been possible to choose an orientation for which $\epsilon = 0$; the interpretation of the observed resonance frequencies under torsional excitation then offers no difficulty.² In recent measurements on metal crystals this has not been possible.^{3,4} The experimental results have been consistent with the assumption that the effective rigidity was G , but a theoretical analysis of the problem seems desirable. The

formulas derived by Goens⁵ are unsatisfactory because in their rigorous form they are inconvenient for numerical calculation, and the first-order correction derived from them is not always reliable.

THEORY

The elastic properties of the specimen are completely described by three quantities E or E' , G or G' , and ϵ . Let E^* and G^* represent whichever values of Young's modulus and the rigidity are chosen for this purpose. Then the actual properties may be regarded as produced by a gradual increase of ϵ from zero to its actual value in an originally isotropic specimen with the same E^* and G^* . The actual frequencies emerge during this process from original unperturbed frequencies which may be classified unambiguously as flexural or torsional but whose values will depend on the meanings of E^* and G^* . Since the "free" frequencies ($E^* = E'$, $G^* = G'$) may be as much as 20 percent lower than the "pure" frequencies ($E^* = E$, $G^* = G$), it is clear that a first-order correction for the perturbation, if it is adequate at all, can be so only when the "unperturbed" frequencies are properly chosen.

In terms of E and G , the differential equations of motion of a cylinder of density ρ and radius a

¹ W. Voigt, *Lehrbuch der Kristallphysik* (Teubner, 1928), pp. 638, 734, 738.

² F. Rose, *Phys. Rev.* **49**, 50 (1936); M. Durand, *Phys. Rev.* **50**, 449 (1936).

³ S. L. Quimby and S. Siegel, *Phys. Rev.* **54**, 293 (1938).

⁴ S. Siegel, *Phys. Rev.* **57**, 537 (1940).

⁵ E. Goens, *Ann. d. Physik* **15**, 455 and 902 (1932). See also R. Kimura, *Proc. Phys.-Math. Soc. Japan* **21**, 686 (1939).

may be written⁶

$$\rho\ddot{\phi} = -\frac{1}{4}a^2E\partial^4\phi/\partial z^4 + 2C\partial^2\psi/\partial z^2, \quad (2)$$

where

$$\rho\ddot{\psi} = -\frac{1}{4}a^2C\partial^4\phi/\partial z^4 + G\partial^2\psi/\partial z^2, \quad (3)$$

$$C = (\epsilon EG/2)^{\frac{1}{2}}.$$

(Here rotatory inertia about the transverse axis *Oy* has been neglected.) The variables ϕ and ψ are the bending and twisting moments exerted across a cross section, divided by the moments of inertia $\frac{1}{4}\pi a^4$ and $\frac{1}{2}\pi a^4$ of the cross section about the corresponding axes. These are more convenient variables than the transverse displacement and angular twist because they make it possible to write the boundary conditions in a form not containing ϵ . For a rod with free ends at $z = \pm l/2$ the boundary conditions are

$$\phi = \psi = 0, \quad \partial\phi/\partial z = 0; \quad (4)$$

only this case will be considered in detail.

The differential Eqs. (2) may be written in three other forms, corresponding to other choices of E^* and G^* ; these may be obtained from (2) by means of (1). If E^* and G^* are held constant but ϵ is set equal to zero, the equations reduce to the form for isotropic specimens, and for vibrations of frequency $p/2\pi$

$$\rho p^2\phi = \frac{1}{4}a^2E^*\partial^4\phi/\partial z^4, \quad \rho p^2\psi = -G^*\partial^2\psi/\partial z^2. \quad (5)$$

The corresponding flexural frequencies $p_i^*/2\pi$ and torsional frequencies $\omega_j^*/2\pi$ are given by⁷

$$p_i^* = n_i^2 \frac{\pi^2 a}{l^2} \left(\frac{E^*}{\rho} \right)^{\frac{1}{2}}, \quad \omega_j^* = j \frac{\pi}{l} \left(\frac{G^*}{\rho} \right)^{\frac{1}{2}}; \quad (6)$$

j is an integer, and n_i is the i th nonvanishing root of

$$\tanh^2(n\pi/2) = \tan^2(n\pi/2) \quad (7)$$

($n_1 = 1.506$, $n_i = i + \frac{1}{2}$ to four figures for $i > 1$). If the frequencies are plotted logarithmically as functions of specimen length l , the torsional frequencies lie on straight lines of slope -1 and the flexural on lines of slope -2 ; these are the fine lines (both solid and dashed) in Fig. 1. The free frequencies ($E^* = E'$, $p_i^* = p_i'$ etc.) are lower than the pure ($E^* = E$, $p_i^* = p_i$ etc.) in the ratio $(1 - \epsilon)^{\frac{1}{2}}$.

⁶ Reference 1, p. 673, or reference 5.

⁷ H. Lamb, *Dynamical Theory of Sound* (Arnold, 1910), p. 124.

The normalized eigenfunctions ϕ_i , ψ_j corresponding to p_i^* and ω_j^* are

$$\phi_i = l^{-\frac{1}{2}} \left[\cosh k_i z / \cosh(k_i l / 2) - \cos k_i z / \cos(k_i l / 2) \right], \quad i \text{ odd}, \quad (8)$$

$$= l^{-\frac{1}{2}} \left[\sinh k_i z / \sinh(k_i l / 2) - \sin k_i z / \sin(k_i l / 2) \right], \quad i \text{ even};$$

$$\psi_j = (2/l)^{\frac{1}{2}} \cos j\pi z / l, \quad j \text{ odd}, \quad (9)$$

$$= (2/l)^{\frac{1}{2}} \sin j\pi z / l, \quad j \text{ even};$$

$$k_i = n_i \pi / l. \quad (10)$$

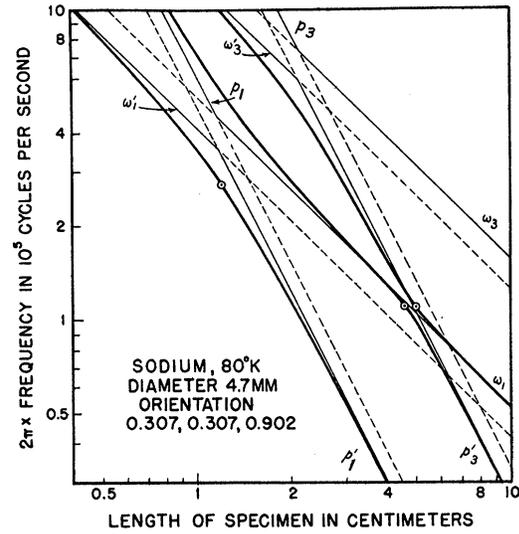


FIG. 1. Unperturbed and perturbed torsional and flexural frequencies for a hypothetical sodium crystal cylinder of the diameter used by Quimby and Siegel, with specimen axis in an orientation for which the coupling between torsion and bending is large. $E = 5.47 \times 10^{10}$, $G = 2.804 \times 10^{10}$ dyne/cm², $\epsilon = 0.3628$. The fine solid and dashed lines represent the unperturbed frequencies as functions of specimen length: the p 's are flexural, the ω 's torsional; the primed are "free," the unprimed "pure." Of these, the ones represented by solid lines are a better approximation to the actual frequencies, which are given by the heavy curves and the circles. The circles have been calculated by a rigorous but laborious method, the curves by the approximate methods of this article. The subscripts are the number of moment loops in the specimen; the strongest interaction is between torsional and flexural modes of vibration for which this number is the same.

The solution for $\epsilon \neq 0$ may be expressed in the form

$$\phi = \sum_i A_i \phi_i, \quad \psi = \sum_j B_j \psi_j. \quad (11)$$

Equations determining the A_i 's and B_j 's may be found by substituting (11) in (2) (with $\partial^2/\partial t^2 = -p^2$), using the differential equations satisfied by the ϕ_i 's and ψ_j 's, multiplying the first of the resulting equations by ϕ_k and the second by ψ_l , and integrating over the length of the

specimen. This gives

$$\begin{aligned} (p^2 - p_k^2)A_k - (2C/G) \sum_j c_{kj} \omega_j^2 B_j &= 0, \\ -(C/E) \sum_i p_i^2 c_{il} A_i + (p^2 - \omega_l^2) B_l &= 0, \end{aligned} \quad (12)$$

where

$$c_{ij} = \int_{-l/2}^{l/2} \phi_i \psi_j dz. \quad (13)$$

For i and j both even or both odd,

$$|c_{ij}| = (4\sqrt{2}/\pi) n_i^2 j / (n_i^4 - j^4); \quad (14)$$

the other c_{ij} 's vanish. Thus Eqs. (12) break up into two sets. One set contains only odd i 's and j 's and refers to modes of vibration in which ϕ and ψ are symmetrical about $z=0$ (see Fig. 2); the other contains only even i 's and j 's and refers to antisymmetrical modes. There is no interaction between a flexural mode of one type and a torsional mode of the other type.

From (14), $c_{11} = 0.972$, $c_{22} = 0.952$, $c_{33} = 0.919$, \dots , $c_{jj} \rightarrow 0.810$ as $j \rightarrow \infty$; and since $\sum_i c_{ij}^2 = \sum_j c_{ij}^2 = 1$, the other c_{ij} 's are small. Therefore a torsional mode interacts chiefly with the flexural mode for which the number of moment loops in the specimen is the same ($i=j$, Fig. 2), and only weakly with the others. As a first approximation, account may be taken of this strongest interaction alone by setting $|c_{ij}| = 1$ for $i=j$, $=0$ otherwise. Then Eqs. (12) separate into pairs; the k th pair contains only A_k and B_k , and for non-vanishing values of these

$$(p^2 - p_k^2)(p^2 - \omega_k^2) - \epsilon p_k^2 \omega_k^2 = 0, \quad (15)$$

whence $p^2 = p_k^2$ or ω_k^2 for $p_k^2 \gg \omega_k^2$, and $p^2 = p_k^2$ or ω_k^2 for $p_k^2 \ll \omega_k^2$. Thus if the strongly interacting frequencies are not too close together, the effect of their interaction is that the lower of them is approximately free and the upper approximately pure. These frequencies correspond to the fine *solid* lines in Fig. 1.

To obtain a better approximation, the best choice of unperturbed frequencies is p_i and ω_i' for lengths below that at which the frequency under consideration and its strongest perturbing frequency become equal; p_i' and ω_i for lengths above this. The fact that the lengths actually used in the experiments lie in the latter range explains the success of the pure torsion formula. The following corrections to the unperturbed frequencies may be derived by standard methods

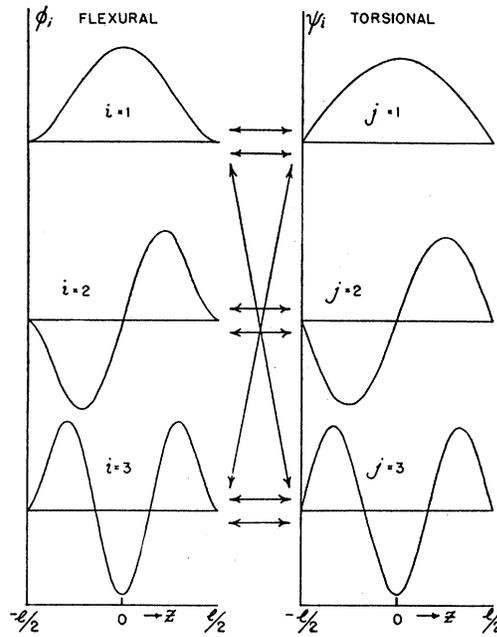


FIG. 2. Unperturbed flexural and torsional modes of vibration and relative degrees of interaction between them ϕ is proportional to the bending moment and ψ to the twisting moment. The double arrows indicate strong interaction, the single arrows weak interaction.

from the equations that now replace (12); the range in which each formula is to be used will be evident from the frequencies occurring in it.

Very near a perturbing frequency, provided the effect of other perturbing frequencies is negligible,

$$p^2 = \frac{1}{2} [b \pm (b^2 - 4c)^{1/2}],$$

where

$$b = p_i'^2 + \omega_j^2 + \eta c_{ij}^2 p_i'^2 \quad (16)$$

or

$$b = p_i^2 + \omega_j'^2 + \eta c_{ij}^2 \omega_j'^2,$$

and

$$\begin{aligned} c &= p_i'^2 \omega_j^2 = p_i^2 \omega_j'^2, \\ \eta &= \epsilon / (1 - \epsilon). \end{aligned}$$

Far from all perturbing frequencies,

$$\begin{aligned} (p^2 - \omega_j^2) / \omega_j^2 &= \eta \sum_i c_{ij}^2 p_i'^2 / (\omega_j^2 - p_i'^2), \\ (p^2 - p_i'^2) / p_i'^2 &= \eta \sum_j c_{ij}^2 p_i'^2 / (p_i'^2 - \omega_j^2), \\ (p^2 - \omega_j'^2) / \omega_j'^2 &= \eta \sum_i c_{ij}^2 \omega_j'^2 / (\omega_j'^2 - p_i^2), \\ (p^2 - p_i^2) / p_i^2 &= \eta \sum_j c_{ij}^2 \omega_j'^2 / (p_i^2 - \omega_j'^2). \end{aligned} \quad (17)$$

Occasionally it is necessary to take account simultaneously of two perturbations, one due to a weakly interacting frequency too close for use of

(17), the other to a strongly interacting frequency still not distant enough to neglect. This is true for instance in Fig. 1 of frequencies produced by interaction of ω_1 and p_3' near their crossing point, where p_1' and ω_3 still produce a considerable effect. Formulas for such cases need not be given here; in the application to experiments the unfavorableness of such a situation is evident without detailed calculation.

APPLICATION

In the experiments mentioned, the specimen is joined end-to-end to a quartz crystal equipped with electrodes, and torsional vibrations are excited piezoelectrically. The frequencies observed are the resonance frequencies of this composite system, but the lengths are so chosen that the junction of the two cylinders is approximately a moment node for torsion. The frequencies are therefore almost the same as the natural frequencies of vibration of the specimen, as long as there is no torsion-flexion coupling. The effect of such coupling on the observed frequencies cannot be computed accurately by using the formulas derived above for the effect on the natural frequencies of the specimen by itself. If, however, that calculation shows that the natural frequency of the specimen alone differs negligibly from the "pure" frequency, it is safe to assume that the observed frequency also differs negligibly from the one that would be observed if bending could be prevented.

The simplest procedure is therefore the following. From the observed frequencies, the elastic constants may be computed by means of the pure torsion formula; the values obtained will be at least approximately correct. From the elastic constants, the unperturbed frequencies may be calculated and plotted as in Fig. 1, for each specimen used. An inspection of the plot will reveal whether any of the experimental points fall in a range where the error is likely to be excessive, and in such ranges the error for a single free rod can be calculated by the formulas given above. Points for which the error is objectionably large may be rejected and the elastic constants recomputed without them; or the whole preliminary measurement and calculation may be used merely as a means of selecting specimen lengths for the final set of measurements.

Figure 1 has been calculated for a hypothetical sodium specimen in a particularly unfavorable orientation, from the values of the elastic constants given by Quimby and Siegel.^{3,8} The heavy curves are corrected frequencies of free vibration. These have been calculated by the method of this article. The circles are check points computed by means of a rigorous formula similar to that of Goens; this calculation consists in solving a cubic equation for some value of p , calculating and plotting a function f of the three roots and of p and l for a number of values of l , and thus finding a combination of l and p for which $f=0$. The calculation for given l would be still more laborious.

It can be seen that the fundamental torsional frequency is practically identical with the unperturbed "pure" frequency for lengths greater than 3 cm, except when the perturbing frequency is very close; in this case two response frequencies would probably be observed and the data would automatically be rejected.⁹ The only possibility of serious error, therefore, lies in the use of too short a length. For the lengths used by Quimby and Siegel one would expect the pure torsion formula to hold quite well, as they found it did. The length range for which the *free* torsion formula would be valid is of no interest, at least for specimens of this diameter, for at such short lengths the specimen can no longer be regarded as thin ($a^2 \ll l^2$).

Siegel in his torsional measurements on copper-gold crystals used two specimens.^{4,10} One had an orientation so close to [100] that the frequency correction at room temperature is only 0.004 percent. In the other ω_2 , which was measured, was rather close to p_4' and was still appreciably perturbed by p_2' ; the effects are 0.7 percent and 0.3 percent, respectively, and additive. The analogous situation in Fig. 1 is a measurement of ω_1 at about $l=6$. Here a correct choice of E^* and G^* is essential; for if p_3 instead of p_3' is chosen as unperturbed frequency, the perturbation is shifted to the right and the whole calculation is erroneous.

⁸ For cubic crystals, in the notation of reference 3, $1/E' = s_{11} - 2s\Gamma$, $1/G' = s_{44} + 4s\Gamma$, $\epsilon = 2s^2E'G'(\Gamma - 4\Gamma^2 + 3\chi)$.

⁹ Reference 3, footnote 12.

¹⁰ The data required for this calculation were kindly provided by Dr. Siegel.