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ANALYSIS OF BOND QUALITY BY RESONANT ULTRASOUND*

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INTRODUCTION

Analysis of the response of small samples of materials to mechanical excitations at ultrasonic frequencies (resonant ultrasound spectroscopy, or RUS) can yield much information about the sample, including its geometry, density (densities, if composite), and elastic constants.⁽¹⁻⁵⁾ In this paper, we sketch the experimental technique, the method by which the data can be analyzed, and extend the analysis to samples which comprise two different materials bonded together. In the latter case the technique can give information about the composition of the sample and bond integrity (i.e. whether or not displacements and stresses are continuous across the interface). Comparison of calculated with measured frequencies for a bonded sample will be made.

RESONANT ULTRASOUND: THE EXPERIMENTAL TECHNIQUE

The setup is sketched in Fig. 1. The sample, which can be a single crystal, isotropic, or composite, is grown or ground to a rectangular parallelepipedal shape (of the order of 1-2 mm on a side) with faces parallel to crystalline planes, if any. It is suspended by opposite corners between two transducers (about 1000 dynes force along the body diagonal hold it in place), one of which is excited at ultrasonic frequencies (usually between 400 and 4000 kHz), and the response of the sample is picked up by the other.

Fig.1 Schematic RUS setup. The sample, a rectangular parallelepiped which may have complicated inhomogeneities, is suspended along a body-diagonal between transmitter and receiver transducers and the input frequency is swept through a given range.

The transmitter frequency can be swept through an appropriate range, so that measurement and analysis together can provide a one-shot determination of many material properties. A typical excitation function comprises a set of very sharp lines centered near the normal-mode frequencies of the elastic vibrations of the sample. The quality factors Q ($=$ full-width at half-maximum/frequency) can range from about 1000 to 40,000. Analysis of the normal-mode frequencies can yield, if the sample is a single crystal, all the elastic constants. This has been done for orthorhombic crystals, with 9 independent moduli, and in principle it will work for a general crystal with 21 elastic constants.

The temperature of the whole system can be accurately controlled and monitored (and it has been, from 4K to above room temperature), so that elastic constants of interesting materials can be measured through various phase transitions.

METHOD OF COMPUTATION

Figure 2 shows a sample comprising an elastic material with general shape, density ρ and elastic constants C_{ijkl} dependent on position. The material occupies the volume V ; its surface is denoted by S . The following felicitous facts facilitate a serendipitous calculation of the normal mode eigenvalues and eigenfunctions for the elastic vibrations of this object. The computational method works for any shape sample, any density variation or anisotropy or inhomogeneity in elastic constants, as long as the sample remains elastic.

Fig. 2 The elastic material occupies V interior to the surface S , on which stress-free boundary conditions are satisfied. The density ρ and the elastic constants C_{ijkl} have arbitrary position dependence inside V .

First we form the Lagrangian density $L = KE - PE$, where the kinetic energy density is

$$KE = \frac{1}{2} \rho \omega^2 u_i u_i$$

(ω is the angular frequency of the assumed overall harmonic time-dependence.) The potential energy density is

$$PE = \frac{1}{2} C_{ijkl} u_{i,j} u_{k,l}$$

(Here we use a summation convention and subscripts following commas denote differentiation). Now we get $\mathcal{L}$ by integrating L over V :

$$\mathcal{L} = \int_V (KE - PE) dV$$

If one then asks what the first-order change in $\mathcal{L}$ is for an arbitrary change in the displacement vector

$$u_i \rightarrow u_i + \delta u_i,$$

the answer is

$$\delta \mathcal{L} = \int_V (\text{Elastic Wave Equation})_i \delta u_i dV - \int_S (\text{Surface Traction})_i \delta u_i dS,$$

plus terms of higher order in δu_i . (The interested reader can easily demonstrate this. It involves one integration by parts.)

Thus the extrema of $\mathcal{L}$ occur at points in the displacement function space which are solutions of the elastic wave equation in V and which satisfy free boundary conditions on S ! This mathematical fortuity must be the result of a serious lapse in Murphy's vigilance.

The following simple method for computing normal modes is thereby suggested. First expand the displacement vector u_i in some complete set of basis functions $\Phi_\alpha(r)$

$$u_i = \sum_{\alpha=1}^L a_{i,\alpha} \Phi_\alpha(r) \quad (i=1,2,3),$$

where the sum is truncated at some limit denoted by L , determined by the desired accuracy, computer capacity, speed and the time one is willing to spend. Then the Lagrangian functional $\mathcal{L}$ can be written

$$\mathcal{L} = 1/2 \omega^2 a^T K a - 1/2 a^T \Gamma a,$$

where

$$K_{i\alpha, i'\alpha'} = \delta_{ii'} \int_V \Phi_\alpha(r) \rho(r) \Phi_{\alpha'}(r) dV$$

and

$$\Gamma_{i\alpha, i'\alpha'} = \int_V \Phi_{\alpha, j}(r) C_{ijij'}(r) \Phi_{\alpha', j'}(r) dV$$

Since $\mathcal{L}$ attains an extremum at the solution we seek, we can find the normal modes of elastic vibration by finding the roots of its derivatives with respect to the components of the $3L$ -dimensional vector a . This gives the generalized eigenvalue equation

$$\omega^2 K a = \Gamma a. \quad (1)$$

If we were to choose Φ to be a set orthonormal with respect to the weight function $\rho(r)$, then K would be the unit matrix, and (1) would reduce to an ordinary eigenvalue equation. But $\rho(r)$ varies from problem to problem, and the moderate penalty in increased computer time which is exacted by a non-diagonal (but symmetric and positive-definite) K is more than compensated by the simplicity of algebra bought by the simple-minded choice of Φ_α which we actually make, namely

$$\Phi_\alpha = \Phi_{lmn}(r) = x^l y^m z^n.$$

Then if the sample is as shown in Fig. 3, namely, a rectangular parallelepiped of elastic material which is homogeneous except for a discontinuity at $z=b$ (below and above which the density and moduli are ρ_1, C_1 , and ρ_2, C_2 respectively), the matrix elements of K and Γ are trivial to compute.

Fig. 3 A rectangular parallelepipedal open-faced sandwich. Material 1 occupies the part of V with $z < b$, material 2 has $z > b$. The origin is at the center of the block.

SYMMETRY

Requirements for computer time and capacity are greatly reduced by the fact that the sample is symmetric under $x \rightarrow -x$ and $y \rightarrow -y$. For a moment let us also assume symmetry under $z \rightarrow -z$, a constraint to be relaxed later.

Now let $\lambda = (-1)^l$, $\mu = (-1)^m$, and $\nu = (-1)^n$. Then a given Φ_{lmn} is characterized by a parity, for example $(++)$ if $l=2, m=3$, and $n=4$. It is easy to see that if the parity of u_1 is $(\lambda\mu\nu)$, it is connected by Γ and K only to certain parities of u_2 and u_3 , so that the matrices are block-diagonal, with each block

characterized by a given triplet of $(\lambda\mu\nu)$'s. The parities of the three components of u are given by

$$\begin{aligned} u_1 &: (-\lambda\mu\nu) \\ u_2 &: (\lambda-\mu\nu) \\ u_3 &: (\lambda\mu-\nu) \end{aligned}$$

There are clearly 8 blocks. In the inhomogeneous case we are interested in here, though, there is no conservation of z -parity, and Γ decomposes into only 4 diagonal blocks. We label them with an integer k as follows;

$$\begin{aligned} u_1 &: (++) \quad (+-) \quad (-+) \quad (- -) \\ u_2 &: (- -) \quad (-+) \quad (+-) \quad (++) \\ u_3 &: (-+) \quad (--) \quad (++) \quad (+-) \\ k &= 1 \quad 3 \quad 5 \quad 7 \end{aligned}$$

RESTRICTIONS

We restrict the sum of orders of Φ by requiring $l+m < n_{xy}$, $n < n_z$. If $(n_{xy}, n_z) = (7, 7)$, the largest of the 4 blocks is 260×260 , the Cray 1 runtime is 10 sec, and the accuracy of the lowest 50 frequencies is 0.1% or better.

Also restricted will be the number of independent elastic constants, just for the sake of simplicity, not to speed up the computation. We will assume the upper part of the sample to be isotropic with Lamé parameters λ_2, μ_2 , and the lower part to have λ_1, μ_1 . Thus the 4-subscript C-tensor has the nonvanishing elements

$$\begin{aligned} C_{1111} &= C_{2222} = C_{3333} = \lambda + 2\mu \\ C_{1212} &= C_{1313} = C_{2323} = \mu \\ C_{1122} &= C_{1133} = C_{2233} = \lambda \end{aligned}$$

TEST CASE

If the densities and elastic constants scale as follows;

$$(\lambda, \mu, \rho)_1 = \alpha (\lambda, \mu, \rho)_2$$

then clearly the frequencies for the case $b = -d_3$ will be the same as those for $b = +d_3$ (all material 1, all material 2), but will vary for intermediate values. This

Fig. 4. $k=7$ normal-mode frequencies of a sample with proportional densities and elastic constants with $\alpha = 5$. Abscissa = fraction of material 1 = $(b + d_3) / 2d_3$, $-d_3 < b < d_3$.

is illustrated for the $k=7$ modes of a sample with $a=5$ on Fig. 4. At the right side the sample is all light and soft; at the left it's all heavy and stiff. The normal modes are the same in these limits. In between some interesting things happen; for example the second and third levels seem to cross once near 100% light, then avoid crossing near 70%.

BONDED SAMPLE

The bonded sample which has been measured experimentally is one which is an alloy (90%Ti,6%Al,4%Va) with a thin layer of Ta bonded onto one face. As input for our program we need the densities and Lamé parameters for materials 1 and 2. λ , μ , and ρ for Ta and pure Ti can be obtained from data given in the AIP Handbook.⁽⁶⁾ For the Ti alloy we obtain them by analyzing RUS for a sample without the Ta layer, resulting in the following values.

	λ	μ	ρ
Ta	1.61	0.67	16.6
pure Ti	0.78	0.44	4.35
Ti alloy	0.40	0.43	4.39
	erg/cm ³	erg/cm ³	g/cm ³

The low frequencies in RUS are often quite insensitive to λ ; thus we can't determine λ well, but it has little effect on the value of b anyway. On the other hand, RUS determines μ quickly and easily to better than 0.5%.

From the densities and dimensions we deduced the thickness of Ta layer to be 4% of $2d_3$. The RUS can also yield this information. Fig. 5 is the $k=3$ RUS for our bonded sample (solid lines connecting the computed points) as a function of thickness of the Ta layer. The dashed lines are the measured RUS. The lowest frequency is apparently a $k=3$ line; because of its small slope there is considerable uncertainty in the Ta thickness it implies, but it is not inconsistent

Fig. 5 Computed $k=3$ spectrum for a Ti alloy sample with a layer of Ta bonded to one side. The lower lines of the spectrum are consistent with the known thickness of Ta and the assumption of a perfect (continuous displacements and stresses) bond. The dashed lines are the measured normal mode frequencies.

with the 2 mil thickness implied by the composite density. To avoid unnecessary clutter we have not plotted the RUS for the other k values. There are, above the first three lines, more computed frequencies than measured ones, but there are many reasons why some resonances might be experimentally invisible. The lowest three lines correspond unambiguously to computed ones, the first and third to $k=3$, the second to $k=5$.

CONCLUSIONS

We have demonstrated that RUS can be used to deduce the thickness of one layer in a bonded sample. There is reason for optimism about the prospect that RUS can tell much about bonded samples. In particular it can tell one whether or not the bond is sound, where it is, and, in principle, what the dimensions and the parameters of the individual components are. Extension of the work to exploit the potential of going beyond a binary bond judgement (perfect/imperfect) to actually gauge bond integrity and strength would be more computationally intensive than that done so far, but in principle it is undoubtedly possible (but maybe not for a mathematician⁽⁷⁾). Thus complete information about shape, size, density and elastic constant variations for composite samples could be obtained from RUS measurements.

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REFERENCES

1. Ichiro Ohno, Shigeru Yamamoto, Orson L. Anderson, and Jiro Noda. J. Phys. Chem. Solids 47, 1103 (1986)
2. Harold H. Demarest, Jr. J. Acoust. Soc. Am. 49, 768 (1969)
3. Ichiro Ohno J. Phys. Earth 24, 355 (1976)
4. A. Migliori, William M. Visscher, S.E. Brown, Z. Fisk, S.-W. Cheong, B. Alten, E.T. Ahrens, K.A. Kubat-Martin, J.D. Maynard, Y. Huang, D.R. Kirk, K.A. Gillis, H.K. Kim, and M.H.W. Chan. Phys. Rev. B41, 2098 (1990)
5. A. Migliori, William M. Visscher, S. Wong, S.E. Brown, I. Tanaka, H. Kojima, and P.B. Allen. Phys. Rev. Letters 64, 2408 (1990)
6. American Institute of Physics Handbook. Third Edition (McGraw-Hill, 1972)
7. M. Kac, "Can one hear the shape of a drum?" . Amer. Math. Monthly 73, 1 (1966)

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