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Free-vibration acoustic resonance of orthorhombic crystals under high-pressure
斜方晶結晶に対する共鳴周波数の圧力依存性解析

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1. Introduction

Free-vibration acoustic resonance (FVAR) of solid is a classical subject studied since the era of L. Rayleigh and W. Ritz [1,2]. Recently, a part of the generalization is conducted by one of the authors [3]. This study considered geometrically nonlinear hyperelastic material, rather than the conventional linear one, and revealed the existence of *color symmetry* embedded in nonlinear FVAR. Although the theory predicts attractive nonlinear phenomena, such as the emergence of color symmetry, higher harmonics generation and amplitude dependence of resonance frequencies, the analysis is limited to two-dimensional and isotropic hyperelastic materials as it requires a considerable amount of computational resources. Recently, we revised the theory on the basis of *quasiharmonic approximation*. Because of the theoretical simplicity, we could evaluate the effect of geometrical and material nonlinearities on FVAR of a three-dimensional and anisotropic hyperelastic material. This study also suggested that we can determined the third-order elastic constants from experimentally measured FVAR frequencies at high pressures. However, the revised theory is still limited to cubic-symmetry crystals and further generalization is needed for practical experiments. The aim of this study is to develop the theory of *quasiharmonic FVAR* for orthorhombic-symmetry crystals.

2. Theory of quasiharmonic FVAR

2.1 Variational formulation

We consider a rectangular parallelepiped-shaped hyperelastic material $\Omega = \{x_i | -L_i/2 < x_i < L_i/2\,, i = 1,2,3\}$, which has a orthorhombic crystal type elastic anisotropy. Let $u_i = u_i(x_i, t)$ be the displacement function expressed by the Lagrange description. Then, nonlinear strain energy density $\mathcal{W}$ is given by

$$\mathcal{W} = \frac{1}{2} C_{ijkl} E_{ij} E_{kl} + \frac{1}{6} C_{ijklmn} E_{ij} E_{kl} E_{mn} + \cdots,$$

where C_{ijkl} and C_{ijklmn} are the second- and third-order elastic constants and E_{ij} is the Green-Lagrange strain tensor. In the present study, we assumed the orthorhombic-symmetry for C_{ijkl} and C_{ijklmn}. Let n_i be the surface normal vector defined on the domain surface $\partial\Omega$ and $g_i = g n_i$ be the external hydrostatic pressure vector applied on the domain. Then, the potential energy is defined as an integration of inner product $\langle g n_i, u_i \rangle$ over $\partial\Omega$. Consequently, the total potential energy W due to the displacement u_i is given by the functional

$$W(u_i) = \int_\Omega \mathcal{W}(u_{i,j}) \mathrm{d}V - \int_{\partial\Omega} \langle g n_i, u_i \rangle \mathrm{d}A.$$

According to continuum mechanics, the kinematic energy T can be expressed by

$$T(u_i) = \int_\Omega \mathcal{T}\left(u_{i,t}\right) \mathrm{d}V, \qquad \mathcal{T} = \frac{1}{2} \rho \left(u_{1,t}^2 + u_{2,t}^2 + u_{3,t}^2\right),$$

where $\rho = \text{const.}$ is the mass density defined on the reference configuration and $\mathcal{T}$ is the kinematic energy density. Then, the action integral I is defined as an integration of the Lagrangian $L = T - W$ over a certain time interval $t \in (0, 2\pi/\omega)$ such that

$$I(u_i) = \int_0^{\frac{2\pi}{\omega}} \left[\int_\Omega (\mathcal{T} - \mathcal{W}) \mathrm{d}V + \int_{\partial\Omega} \langle g n_i, u_i \rangle \mathrm{d}A \right] \mathrm{d}t,$$

where ω is the resonant frequency. According to the principle of stationary action, the actual displacement u_i must satisfy the stationary condition $\delta I = 0$, where δI stands for first variation of action integral.

2.2 Direct analysis by Ritz method

We solve the variational problem $\delta I = 0$ directly by using the Ritz method. First, we expand the displace function into the *quasiharmonic* form:

$$u_i(x_i, t) = \alpha x_i + \sum_{s=1}^{S} a_{i,s} \phi_s(x_i) \cos \omega t,$$

where ϕ_s consists of the normalized Legendre polynomial $\bar{P}_s$ of the order s. Here, the first term shows the static displacement, which is responsible

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for a uniform contraction (or expansion) by the external pressure P. The second is responsible for the harmonic vibration. Nonlinear interaction between the static and harmonic displacements yield the vibration to be quasiharmonic.

3. Resonant vibration under high-pressure

3.1 Amplitude and pressure dependence of FVAR frequency

Figure 1 (left) shows the amplitude dependence of FVAR frequency ω_i of Magnesium, which has a hexagonal symmetry, obtained at $P = 0$. As seen here, the frequencies show monotonic decreasing on the order of 10^{-8}. The right figure shows the normalized pressure dependence of ω_i. This result indicates that the pressure dependence varies with the vibration mode and it has a strong linearity in the present pressure range: $P < |10|$ MPa.

3.2 Mode Grüneisen parameter

According to Fig. 1(left), we can approximate the pressure dependence of FVAR frequency by a linear function $\omega_i(P) = \psi_i P + \omega_i(0)$. Using the thermodynamic relation, the pressure derivative ψ_i can be transformed into the mode Grüneisen parameter γ_i such that:

$$\gamma_i := -\frac{\mathrm{d}\ln\omega_i}{\mathrm{d}\ln V} = -\frac{V}{\omega_i}\frac{\mathrm{d}\omega_i}{\mathrm{d}V} = -\frac{V}{\omega_i}\frac{\mathrm{d}\omega_i}{\mathrm{d}P}\frac{\mathrm{d}P}{\mathrm{d}V} = -\frac{\psi_i}{\omega_i}B,$$

where B stands for the bulk modulus. Figure 2 plots γ_i with respect to the FVAR frequency $\omega_i(0)$ for the first to 2,000th modes. Although γ_i exhibits large fluctuations at the low-frequency side, the fluctuation diminishes at high-frequencies and converge to a specific value. Hence, we approximate the behavior by a double exponential function and determined the high-frequency limit. Table 1 summarizes the result. For comparison, we included the Grüneisen parameter estimated from Debye model. As seen in the table, agreement between the two models is fairly well.

Table 1 The high-frequency limit mode Grüneisen parameter γ^{∞}.

element	this work	Debye model
Mg	1.48	1.58
Ti	1.83	1.97
Zr	1.77	1.91
Hf	1.67	1.90

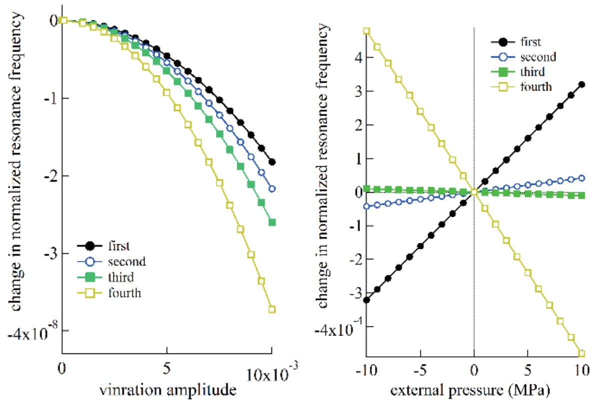

Fig. 1 Amplitude dependence (left) and pressure dependence (right) of the normalized frequency obtained from Mg.

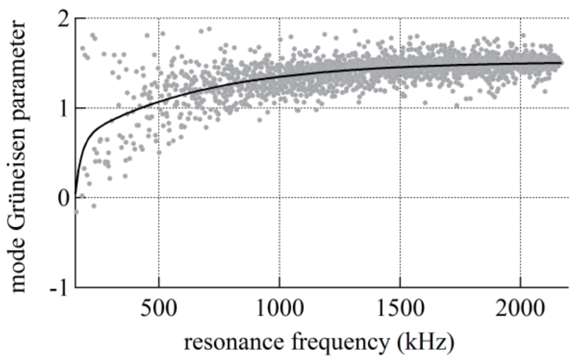

Fig. 2 Mode Grüneisen parameter γ_i plotted as a function of FVAR frequency $\omega_i(0)/2\pi$.

4. Conclusions

We developed the theory of *quasiharmonic FVAR* for orthorhombic-symmetry crystals. Numerical analysis revealed that the FVAR frequencies depend linearly on the pressure and the slopes vary with the vibration modes. We estimated the high-frequency limit mode Grüneisen parameters γ^{∞} from least-squares fitting of γ_i to a double exponential function. The limits γ^{∞} showed quantitative agreement with the previously reported ones. This result verify the present theory.

References

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