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 determine 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 \( \Omega = \{ x_i | -L_i/2 < x_i < L_i/2 \}, \) which has an 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

\[
W(u_i) = \int_\Omega \mathcal{W}(u_i) dV - \int_{\partial \Omega} \langle g n_i, u_i \rangle dA.
\]

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

\[
T(u_i) = \int_\Omega T(u_i) dV,
\]

\[
T = \frac{1}{2} \mu \left( u_{xx}^2 + u_{yy}^2 + u_{zz}^2 \right),
\]

where \( \mu \) is the mass density defined on the reference configuration and \( T \) 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

\[
I(u_i) = \int_0^{2\pi/\omega} \left[ \int_\Omega (T - W) dV + \int_{\partial \Omega} \langle g n_i, u_i \rangle dA \right] dt,
\]

where \( \omega \) 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 \( \delta I \) 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:

\[
u_i(x_i,t) = a x_i + \sum_{s=1}^{s} a_i \phi_s(x_i) \cos \omega t,
\]

where \( \phi_s \) consists of the normalized Legendre polynomial \( P_s \) of the order \( s \). Here, the first term shows the static displacement, which is responsible...
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 $\omega_i$ of Magnesium, which has a hexagonal symmetry, obtained at $P = 0$. As seen here, the frequencies show monotonic decreasing on the order of $10^{-4}$. The right figure shows the normalized pressure dependence of $\omega_i$. This result indicates that the pressure dependence varies with the vibration mode and it has a strong linearity in the present pressure range: $P < |10| \text{ MPa}$.

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 $\psi_i$ can be transformed into the mode Grüneisen parameter $\gamma_i$ such that:

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

where $B$ stands for the bulk modulus. Figure 2 plots $\gamma_i$ with respect to the FVAR frequency $\omega_i(0)$ for the first to 2,000th modes. Although $\gamma_i$ 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 $\gamma^{\infty}$.

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<th>element</th>
<th>this work</th>
<th>Debye model</th>
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<tr>
<td>Mg</td>
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<td>1.58</td>
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<td>Hf</td>
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<td>1.90</td>
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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 $\gamma^{\infty}$ from least-squares fitting of $\gamma_i$ to a double exponential function. The limits $\gamma^{\infty}$ showed quantitative agreement with the previously reported ones. This result verify the present theory.

References