Abstract—A numerical approach based on the finite-element method is described for the analysis of periodic waveguides for acoustic waves. The validity of the method is confirmed by comparing the numerical results for the dispersion curves of horizontal shear (SH) waves in a groove grating on an isotropic material with the experimental results. The application of this approach is also demonstrated by investigating the propagation characteristics of SH surface waves in a groove grating on a piezoelectric material, the stop-band width and the center-frequency shift in the dispersion diagram for Rayleigh waves are calculated, which are important parameters for design of a reflector, and the influences of groove shape on these parameters are examined.

I. INTRODUCTION

In recent years, attention has been given to the use of gratings on solid surfaces to reduce the propagation velocity of acoustic waves and to introduce bandgaps and cutoff frequencies into their dispersion relations for the purpose of producing delay lines and filtering devices [1]–[6]. Several methods for the analysis of periodic waveguides in Fig. I have been proposed, and the coupled-mode theory, which derives the coupled-mode equations under the assumption of small perturbations, is widely used [7]–[12]. The calculation procedure of this method is relatively simple, but the accuracy is degraded for large perturbations. On the other hand, it is possible to increase the accuracy by expanding the acoustic and electromagnetic fields in terms of Fourier series by means of the Floquet theorem and deriving the homogeneous linear equations of infinite order [13]–[19]. However, it seems to be difficult to apply this approach to arbitrarily shaped periodic waveguides.

In this paper a numerical approach based on the finite-element method is described for the analysis of arbitrarily shaped periodic waveguides for acoustic waves. The validity of the method is confirmed by comparing the numerical results for the dispersion curves of horizontal shear (SH) waves in a groove grating on an isotropic material with the experimental results [4]. We also demonstrate the application of this approach by investigating the propagation characteristics of SH surface waves in a groove grating on a layered isotropic material. Furthermore, for a groove grating on a piezoelectric material, the stop-band width and the center-frequency shift in the dispersion diagram for Rayleigh waves are calculated, which are important parameters for design of a reflector, and the influences of groove shape on these parameters are examined.

II. BASIC EQUATIONS

The structure under study is periodic in the x direction with period d as shown in Fig. I. The region Ω surrounded by boundaries Γ₁ to Γ₄ is the basic cell. The mechanical boundary conditions on Γ₁ and Γ₄ are \( u_x = u_y = u_z = 0 \) or \( T_{xx} = T_{yy} = T_{zz} = 0 \), where \( u_x, u_y, \) and \( u_z \) are the particle displacements, \( T_{xx}, T_{yy}, \) and \( T_{zz} \) are the stresses, and \( n \) denotes the outward normal direction to the boundary. The electrical boundary conditions on Γ₂ and Γ₃ are \( \Phi = 0 \) or \( D_n = 0 \), where \( \Phi \) is the electric potential and \( D_n \) is the electric displacement.

Assuming that no variation exists in the z direction, we have the following equations [1]:

\[
\frac{\partial T_x}{\partial x} + \frac{\partial T_y}{\partial y} + \omega^2 \rho u = 0 \tag{1a}
\]

\[
\frac{\partial D_x}{\partial x} + \frac{\partial D_y}{\partial y} = 0 \tag{1b}
\]

where

\[
\mathbf{u} = [u_x \ u_y \ u_z]^T
\]

\[
\mathbf{T} = [T_{xx} \ T_{yx} \ T_{xy}]^T
\]

\[
\mathbf{T} = [T_{xx} \ T_{yy} \ T_{zy}]^T
\]

Here \( \omega \) is the angular frequency, \( \rho \) is the mass density, and \( T \) denotes a transpose.

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III. Finite-Element Approach

Dividing the region $\Omega$ into a number of second-order triangular elements in Fig. 1, $u$ and $\phi$ within each element are defined in terms of the particle displacement and the electric potential at the corner and midside nodal points:

$$u = [N]^T \{u\} \quad \text{(3a)}$$
$$\phi = [N]^T \{\phi\} \quad \text{(3b)}$$

where

$$[N] = \begin{bmatrix} [N_x] & [0] & [0] \\ [0] & [N_y] & [0] \\ [0] & [0] & [N_z] \end{bmatrix} \quad \text{(4)}$$

Here $\{u\}$ and $\{\phi\}$ are the particle displacement and electric potential vectors corresponding to the nodal points within each element, respectively, $[N]$ is the shape function vector [20], [21], $[0]$ is a null vector, and $\cdot^T$ denote a column vector and a row vector, respectively.

The well-known constitutive relations for piezoelectric materials are written as [1], [20]

$$T = [c] S - [e]^T E \quad \text{(5a)}$$
$$D = [\varepsilon] E + [e] S \quad \text{(5b)}$$

where $T$, $S$, $D$, and $E$ are the stress, strain, electric displacement, and electric field vectors, respectively, and $[c]$, $[e]$, and $[\varepsilon]$ are the elastic constant, piezoelectric, and permittivity tensors, respectively.

The strain vector $S$ and the electric field vector $E$ are expressed as [20]

$$S = [B_u] \{u\} \quad \text{(6a)}$$
$$E = -[B_\phi] \{\phi\} \quad \text{(6b)}$$

where $[B_u]$ and $[B_\phi]$ are given by

$$[B_u] = \begin{bmatrix} [N_x] & [0] & [0] & [0] & [N_z] \\ [0] & [N_y] & [0] & [0] & [N_z] \\ [0] & [0] & [N_y] & [N_z] & [0] \end{bmatrix} \quad \text{(7a)}$$
$$[B_\phi] = \begin{bmatrix} [N_x] & [N_y] & [0] \end{bmatrix} \quad \text{(7b)}$$

Here $[N_x] = \partial [N] / \partial x$ and $[N_y] = \partial [N] / \partial y$.

Equation (5) is now expressed in terms of $\{u\}$ and $\{\phi\}$ as

$$T = [c] [B_u] \{u\}_e + [e]^T [B_\phi] \{\phi\}_e \quad \text{(8a)}$$
$$D = -[\varepsilon] [B_\phi] \{\phi\}_e + [e] [B_u] \{u\}_e \quad \text{(8b)}$$

Using a Galerkin procedure on (1), we obtain

$$\int_\Omega \{N\} \left( \partial T_x / \partial x + \partial T_y / \partial y + \omega^2 \rho_e u \right) d\Omega = \{0\} \quad \text{(9a)}$$

where the integration is carried over the element subdomain $\Omega_e$.

Integrating by parts, (9) becomes

$$\int_\Omega \left( [N_x] T_x + [N_y] T_y - \omega^2 \rho_e [N] u \right) d\Omega = \{0\} \quad \text{(10a)}$$

$$\int_\Omega \left( \{N_x\} D_x + \{N_y\} D_y \right) d\Omega = \{0\} \quad \text{(10b)}$$

Noting that $T$ and $D$ are continuous across $\Gamma_e$ (boundary conditions at the interface between two different media) and considering the boundary conditions on $\Gamma_3$ and $\Gamma_4$ (See Section II), from (3), (8), and (10) the following global matrix equation is derived:

$$\left[ \begin{array}{c} [K] \quad [C] \\ [C]^T \quad [-G] \end{array} \right] \left[ \begin{array}{c} \{u\} \\ \{\phi\} \end{array} \right] = \omega^2 \left[ \begin{array}{c} [M] \quad [0] \\ [0] \quad [0] \end{array} \right] \left[ \begin{array}{c} \{u\} \\ \{\phi\} \end{array} \right] \quad \text{(11)}$$

where

$$[K] = \sum_e \int_\Omega \int_\Omega [B_u] [c] [B_u]^T dx dy \quad \text{(12a)}$$
$$[C] = \sum_e \int_\Omega \int_\Omega [B_u] [e]^T [B_\phi]^T dx dy \quad \text{(12b)}$$
$$[G] = \sum_e \int_\Omega \int_\Omega [B_\phi] [e]^T [B_\phi]^T dx dy \quad \text{(12c)}$$
$$[M] = \sum_e \int_\Omega \int_\Omega \rho_e [N] [N]^T dx dy \quad \text{(12d)}$$

Here $\{u\}$ is the nodal particle displacement vector, $\{\phi\}$ is the nodal electric potential vector, $[0]$ is a null matrix, and $\Sigma_e$ and $\Sigma'_e$ extend over all different elements and the elements related to the boundaries $\Gamma_1$ and $\Gamma_2$, respectively. Constraints on the stress and the electric displace-
ment on $\Gamma_3$ and $\Gamma_4$ are natural boundary conditions and will be automatically satisfied. Constraints on the particle displacement and the electric potential on $\Gamma_3$ and $\Gamma_4$ may be imposed simply by deleting a row and a column of the relevant element matrices.

The periodic conditions are given by

$$ u \mid _{\Gamma_2} = p u \mid _{\Gamma_1} \quad (13a) $$

$$ T_x \mid _{\Gamma_2} = p T_x \mid _{\Gamma_1} \quad (13b) $$

$$ \phi \mid _{\Gamma_2} = p \phi \mid _{\Gamma_1} \quad (13c) $$

$$ D_x \mid _{\Gamma_2} = p D_x \mid _{\Gamma_1} \quad (13d) $$

where

$$ p = \exp (-j\beta d). \quad (14) $$

Here $\beta$ is the phase constant in the $x$ direction.

Using (13), from (11) we obtain

$$ \begin{bmatrix} [\tilde{K}] & [\tilde{C}] \\ [\tilde{C}]^\dagger & -[\tilde{G}] \end{bmatrix} \begin{bmatrix} \{\tilde{u}\} \\ \{\tilde{\phi}\} \end{bmatrix} - \omega^2 \begin{bmatrix} [M] [0] \\ [0] [0] \end{bmatrix} \begin{bmatrix} \{\phi\} \\ \{\phi\} \end{bmatrix} = \{0\} \quad (15) $$

Here the components of the $\{u\}_1$ and $\{\phi\}_1$ vectors are the values of the particle displacement and the electric potential at nodal points on the boundary $\Gamma_1$, respectively; the components of the $\{u\}_0$ and $\{\phi\}_0$ vectors are the values of the particle displacement and the electric potential at nodal points in the interior region except the boundaries $\Gamma_1$ and $\Gamma_2$, respectively; the matrices $[\tilde{C}]$, $[\tilde{G}]$, and $[M]$ are given by replacing $K$ in (18) by $C$, $G$, and $M$, respectively; * and $\dagger$ denote a complex conjugate and a complex conjugate transpose, respectively; and $[K]_{00}$, $[K]_{01}$, $[K]_{10}$, $[K]_{11}$, $[K]_{20}$, $[K]_{21}$ are the submatrices of $[K]$:

$$ [K] = \begin{bmatrix} [K]_{00} & [K]_{01} & [K]_{02} \\ [K]_{10} & [K]_{11} & [K]_{12} \\ [K]_{20} & [K]_{21} & [K]_{22} \end{bmatrix} \quad (19) $$

Eliminating $\{\phi\}$ from (15), we obtain the following final eigenvalue equation:

$$ ([\tilde{K}] + [\tilde{C}] [\tilde{G}]^{-1} [\tilde{C}]^\dagger - \omega^2 [M]) \{u\} = \{0\}. \quad (20) $$

This equation determines the propagation characteristics of periodic waveguides. In the present analysis, the Cholesky method, the Householder's method, the method of bisections, and the method of inverse iterations are suitably used for solving (20).

**IV. COMPUTED RESULTS**

First, we consider a groove grating on an isotropic material. Fig. 2 shows the dispersion curves of SH waves of an isotropic waveguide with rectangular grooves, where $k_x = \omega/v_x$, and $v_x$ is the bulk shear wave velocity. Our results agree well with the experimental results [4]. Comparison of the results in Fig. 2(a) and (b) shows that the deeper grooves give a greatly increased amount of wave slowing.

Fig. 3 shows the dispersion curve of the fundamental SH surface wave of a layered isotropic waveguide with rectangular grooves, where $k_{11} = \omega/v_{11}$ and $v_{11}$ and $v_{12}$ are the bulk shear wave velocities of the substrate and the film, respectively. The phase velocity of this SH surface wave is lower than that of the fundamental Love wave and, for large $\beta d$, this velocity may become even lower than the bulk shear wave velocity of the film ($v_{12}$).

Next we consider a groove grating on a piezoelectric material ($Y-Z$ LiNbO$_3$) and investigate the stop-band width and the center-frequency shift of the stop band at $\beta d = \pi$ (the first Bragg reflection) in the dispersion diagram for Rayleigh waves. In the case of Rayleigh waves, we set $u_x = u_y = u_z = D_x = 0$ on the boundary $\Gamma_2$ in Fig. 1 [20].

Fig. 4 shows the normalized stop-band width $\Delta F/f_0$ and the normalized center-frequency shift $\Delta f/f_0$ of a piezoelectric waveguide with rectangular grooves, where $\Delta F/f_0$, $\Delta f/f_0$, and $f_0$ are given by

$$ \Delta F/f_0 = (f_u - f_l)/f_0 \quad (21) $$

$$ \Delta f/f_0 = [(f_u + f_l)/2 - f_l]/f_0 \quad (22) $$

$$ f_0 = v_R/2d. \quad (23) $$

Here $f_u$ and $f_l$ are the upper and lower bound frequencies of the stop band, respectively, and $v_R$ is the velocity of the Rayleigh wave on a $Y-Z$ LiNbO$_3$ substrate. In Fig. 4 the groove width is one-half of the period $d$, the groove depth $h$ is varied, and the substrate thickness is about five times the period $d$. Our results for the center-frequency shift agree well with the experimental results [6].

Lastly, we examine the influences of groove shape on the stop-band width and the center-frequency shift of the groove grating on $Y-Z$ LiNbO$_3$. Fig. 5 shows $\Delta F/f_0$ and
Δf/fo at βd = π of a piezoelectric waveguide with trapezoidal grooves (θ ≠ 0), where dashed lines are for the rectangular grooves (θ = 0) and are the same as the solid lines in Fig. 4. It is found from Fig. 5 that the center-frequency shift is decreased as θ becomes larger. This is due to the fact that for large θ, namely, a gentle slope, the energy storage effect [3] becomes smaller. When the area of trapezoidal groove (Sf) is larger than that of rectangular groove (Sr), namely, Sf > Sr in Fig. 5(a), the stop-band width for trapezoidal grooves is smaller than that for rectangular grooves. Also, as θ becomes larger, the stop-band width is decreased. When Sf = Sr in Fig. 5(b), the influence of θ on the stop-band width is extremely small. When Sf < Sr in Fig. 5(c), the stop-band width for trapezoidal grooves is slightly larger than that for rectangular grooves. For very large θ (for example, θ = 80°), however, the stop-band width for trapezoidal grooves becomes smaller than that for rectangular grooves.

V. CONCLUSION

A method of analysis based on the finite-element method was developed for the solution of the propagation problem in periodic waveguides for acoustic waves. Numerical examples are presented for the groove gratings for SH waves and Rayleigh waves. This approach can be easily applied to the metallic gratings [2], [5], [7], [8], [13]–[16], [19].
Fig. 5. Stop-band width and center-frequency shift for Rayleigh wave of piezoelectric waveguide with trapezoidal grooves. (a) $S > S_0$. (b) $S = S_0$. (c) $S < S_0$. ($S_0$ and $S$ are areas of trapezoidal and rectangular grooves, respectively).

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