Adaptive Lagrange finite element methods for high precision vibrations and piezoelectric acoustic wave computations in SMT structures and plates with nano interfaces*

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Abstract: This paper discusses the validity of（adaptive）Lagrange generalized plain finite element method（FEM）and plate element method for accurate analysis of acoustic waves in multi-layered piezoelectric structures with tiny interfaces between metal electrodes and surface mounted piezoelectric substrates. We have come to conclusion that the quantitative relationships between the acoustic and electric fields in a piezoelectric structure can be accurately determined through the proposed finite element methods. The higher-order Lagrange FEM proposed for dynamic piezoelectric computation is proved to be very accurate（prescribed relative error 0.02% – 0.04%）and a great improvement in convergence accuracy over the higher order Mindlin plate element method for piezoelectric structural analysis due to the assumptions and corrections in the plate theories. The converged Lagrange finite element methods are compared with the plate element methods and the computed results are in good agreement with available exact and experimental data. The adaptive Lagrange finite element methods and a new FEA computer program developed for macro- and micro-scale analyses are reviewed，and recently extended with great potential to high-precision nano-scale analysis in this paper and the similarities between piezoelectric and seismic wave propagations in layered structures and plates are stressed.

Key words: Lagrangian finite element，surface mount，resonator structure，plate element，anisotropic piezoelectric quartz material，acoustic wave，computational nano-dynamics，SMT（surface mount technology）
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INTRODUCTION

As we know，the computational piezoelectric dynamic equations for high frequency acoustic wave propagations were originally expanded from the general computational structural mechanics，and the finite element methods（FEM）initially from aerospace and civil engineering. Therefore，the computational dynamics method extended for computational piezoelectricity still remains to be valid for low frequency damaging vibrations in the structures in civil，mechanical，aerospace and other engineering fields if the electric effect is ignored.

However，a layered piezoelectric resonator structure can become smart when it is composed of certain special smart materials. Among them，single crystal materials are classed as piezoelectric quartz crystals because they exhibit the following interesting phenomena：When the quartz crystal is mechanically strained，or when the crystal is deformed by the application of external stress，electric charges appear on certain of the crystal surfaces. Conversely，when a piezoelectric crystal is placed in an electric field，the crystal exhibits strain.

In theory and practice，it is an expensive and challenging task to accurately determine quantitatively the high-frequency relationship and design various high quality piezoelectric BAW and SAW wave devices composed of layered materials and arbitrarily shaped metal electrodes（Hossack et al，1991；Datta，1986）.

Bulk and surface wave modeling analysis has become an interdisciplinary subject，for instance，in earthquake and piezoelectric fields.

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The low frequencies are more damaging and the material properties are usually highly nonlinear in computational geotechnical engineering mechanics (Desi and Zhang, 1998). In piezoelectric BAW and SAW technology, the objective is to precisely generate and control higher frequency acoustic waves in piezoelectric anisotropic elastic substrates where the acoustic fields generate electric fields and vice versa.

Seiko Epson Corporation conducted expensive experiment on ST-cut SAW motion in the micro piezoelectric resonators with quartz crystal substrates, and we have been trying to develop accurate finite element methods and reusable computer programs to guarantee the computational accuracy for various cut angles and increase savings in memory and storage of computers. Besides the finite element methods needed, an efficient eigenvalue solver is also required for solving large-scale piezoelectric devices (Yong et al., 1996). The AT-cut results by piezoelectric plate element method were found to be insufficiently accurate and inconsistent with analytical experimental data (Wang et al., 1999), and are further verified and computationally improved for ST-cut piezoelectric quartz substrates in this work. Similar inaccuracies exist in shell elements (Hong et al., 1999). The inaccuracies were mainly due to assumptions and corrections in plate theories (Mindlin, 1955, 1972, 1984). These errors are not allowed in high accuracy high frequency piezoelectric acoustic wave analysis.

To improve the past work on piezoelectric plate element methods, we have recently tried to use adaptive Lagrange generalized plain strain finite element methods and to model high-frequency piezoelectric acoustic waves in micro-resonator structures. The much higher frequencies and velocities for bulk and surface wave propagations are further studied and computed on a nano-scale in this paper with reliably high accuracies.

FINITE ELEMENT METHODS FOR PIEZOELECTRIC STRUCTURAL DYNAMICS AND ACOUSTIC WAVES IN SOLIDS AND PLATES

The piezoelectric dynamic equations are electro-mechanically coupled and the electric potential corresponds to zero mechanical mass, and the dielectric matrix is singular. Therefore, these piezoelectric dynamic equations require a special accurate finite element method and a large-scale eigenvalue solver.

With dielectric effect introduced, the generalized structural dynamic equations for finite element computation become piezoelectric dynamic ones in this discrete form:

$$\sum_{e=1}^{NE}\left([M]\begin{Bmatrix} q'' \\ \varphi'' \end{Bmatrix} + \sum_{e=1}^{NE}\left([K]\begin{Bmatrix} q \\ \varphi \end{Bmatrix}\sum_{e=1}^{NE}\begin{Bmatrix} F \\ Q \end{Bmatrix}\right.\right. \tag{1}$$

where NE denotes the total number of elements in a structure, M_{uu}, K_{uu}, $K_{u\phi}$ and $K_{\phi\phi}$ are the mechanical mass, mechanical stiffness, piezoelectric coupling and dielectric matrices, respectively, where q, φ, F and Q are the mechanical displacement, electric potential, mechanical force and electric charge vectors, respectively. By setting $M_{uu} = 0$, the piezoelectric dynamics relations in Eq. (1) become static piezoelectric governing equations for surface mount stress prediction.

In the piezoelectric finite element formulation, we have the element mass matrix

$$[M] = \begin{bmatrix} M_{uu} & 0 \\ 0 & 0 \end{bmatrix}, \quad [M_{uu}] = \int_v \rho [N]^{\mathrm{T}} [N] \mathrm{d}v \tag{2}$$

where $[N]$ is the element shape function matrix for the mechanical part, and ρ is the mass density of piezoelectric materials like quartz crystals. For quartz crystal, $\rho = 2650\ \mathrm{kg/cm^2}$ (Datta, 1986, Valpey-Fisher Corp, 1997)

We also have the finite element stiffness matrix and material stiffness matrix respectively,

$$[K] = \begin{bmatrix} K_{uu} & K_{u\phi} \\ K_{u\phi}^{\mathrm{T}} & K_{\phi\phi} \end{bmatrix} = \int_v [B]^{\mathrm{T}} [C][B] \mathrm{d}v \tag{3}$$

$$[C] = \begin{bmatrix} [C_e]_{5\times5} & [P_e]_{2\times5}^{\mathrm{T}} \\ [P_e]_{2\times5} & [D_e]_{2\times2} \end{bmatrix}_{7\times7} \tag{4}$$

where $[C_e]_{5\times5}$, and $[D_e]_{2\times2}[P_e]_{2\times5}$ denote the mechanical stiffness constants, piezoelectric constant and dielectric permittivities, respectively. $[B]$ is the geometric matrix for the finite element method (Zhang et al., 1997). For piezoelectric generalized plain strain finite element method, the matrix is determined by the following element field interpolation and its corresponding generalized element strains:

$$\begin{Bmatrix} U \\ \Phi \end{Bmatrix} = \{u \quad v \quad w \quad \phi\}^{T} = \sum_{i=1}^{nen} N_i \{u \quad v \quad w \quad \phi\}_i^{T} = [N^*]\begin{Bmatrix} q \\ \varphi \end{Bmatrix} \quad (5)$$

where N_i ($i = 1, 2, \cdots$ nen) are the shape functions of an element with nen (Number of elemental nodes) nodes, and the generalized element strains can be expressed as

$$\{\varepsilon^*\} = \{\varepsilon_x \quad \varepsilon_y \quad \gamma_{yz} \quad \gamma_{zx} \quad \gamma_{xy} \quad \phi_{,x} \quad \phi_{,y}\}^{T} = [D][N^*]\begin{Bmatrix} q \\ \varphi \end{Bmatrix} = \mathrm{diag}[D_u, \quad D_\phi][N^*]\begin{Bmatrix} q \\ \varphi \end{Bmatrix} = [B]\begin{Bmatrix} q \\ \varphi \end{Bmatrix} \quad (6a)$$

where $[D_u]$ and $[D_\phi]$ are the differential operators for mechanical and dielectric parts in generalized plain strain and plate theories omitted here for simplicity. In the differential operator, the piezoelectric constraint for the generalized plain strain constitutive model is given as:

$$\frac{\partial(\cdot)}{\partial z} = 0 \quad (6b)$$

The complex equations for high order AT-cut Mindlin plate theory were reviewed by Wang et al. (1999). However, we can see the difference between the plain and plate constitutive models from the 2-*D* mechanical material stiffness matrices:

$$[C_e] = C_0 \begin{bmatrix} 1 & \mu & 0 \\ & 1 & 0 \\ \text{sym.} & & \frac{1-\mu}{2} \end{bmatrix} \quad (7)$$

where μ is Poisson ratio and

$$C_0 = \frac{E}{1-\mu^2} \quad \text{for plane theories} \quad (8a)$$

$$C_0 = \frac{Et^3}{12(1-\mu^2)} \quad \text{for plate problems} \quad (8b)$$

where E and t are Young's modulus and plate thickness respectively. Of course, the constitutive matrices $[C]$ in Eq. (4) and geometric matrix $[B]$ in Eqs. (3) and (6) are more complicated with dielectric and higher order terms included for electro-mechanical or piezoelectric analysis, and for generalized plain strain and higher order plate modeling.

From Eqs. (1-4) we know that the generalized eigenvalue matrix equations for piezoelectric analysis are

$$\begin{bmatrix} K_{uu} & K_{u\phi} \\ K_{u\phi}^{T} & K_{\phi\phi} \end{bmatrix}\begin{Bmatrix} q \\ \varphi \end{Bmatrix} = W^2 \begin{bmatrix} M_{uu} & 0 \\ 0 & 0 \end{bmatrix}\begin{Bmatrix} q \\ \varphi \end{Bmatrix} \quad (9)$$

Because the dielectric matrix $K_{\phi\phi}$ is singular and not on the same scale in value as $[K_{uu}]$, and is $[K]$ expanded with dielectric part and requires a huge amount of computer storage and memory in piezoelectric eigenvalue solution, a special efficient eigen solver is required, as the traditional static-condensed and perturbation methods do not provide accurate eigenvalues (Yong et al., 1996).

Once the finite element computed eigenvalues are obtained, i.e. circular frequency ω, we can easily calculate the wave velocity

$$\text{Wave velocity} = \omega PT/\pi \quad (10a)$$

where PT is half wavelength. For computing the bulk wave frequency, the spectrum is usually normalized by the fundamental thickness-shear frequency:

$$\omega_0 = \frac{\pi}{2t}\sqrt{\frac{c_{66}}{\rho}} \quad (10b)$$

where c_{66} and ρ are material stiffness coefficient and mass density respectively.

The acoustic surface wave velocity is characterized by being always the same in a free-surface structure of a material for any frequencies. For piezoelectric quartz material, the ST-cut SAW wave velocity is always 3158m/s (Datta, 1986).

SELECTION OF FINITE ELEMENT TYPES FOR HIGH-FREQUENCY VIBRATIONS AND ACOUSTIC WAVES

The right choice of finite element types, i.e. $[N]$, is essential to the accurate modeling of high frequency piezoelectric acoustic waves. Ordinary even high order plate elements (Fig. 1a) (Wang et al., 1999; Hong et al., 1999) based on the plate theories (Mindlin, 1955, 1972), and 4-node based finite element methods for improved stress analysis (Zhang et al., 1993, 1997) are numerically proved to be inappropriate for piezoelectric acoustic wave computation. The 9-node Lagrangian finite element method of quadratic type is appropriate for small computers, while the higher order 16-node Lagrangian finite element method can be effectively applied using Unix workstations (Zhang et al., 2002), although adaptive third-order element is rarely adopted in stress prediction (Steward and Chen, 1997). Adaptive Lagrangian finite element methods with inside nodes (Fig. 1b) and error control should be the first choice for the piezoelectric acoustic waves in this paper.

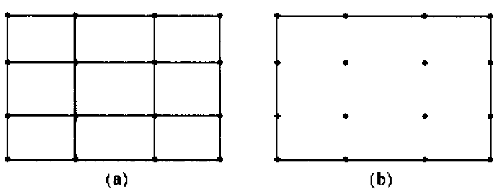

Fig. 1 Third-order plate element and lagrange element methods for vibrations and acoustic waves
(a) DOF per node = 6; (b) DOF per node = 3

Traditionally, the error indicator of the computed stress/strain distribution was adopted in the adaptive FEA for linear problems. For highly nonlinear problems, the computational -constitutive adaptive indicator was proposed for the adaptive finite element analysis (Desai et al., 1998). Unlike the stress analysis in SAW devices, there are no stresses and strains to be computed in the SAW eigenvalue analysis, the frequencies and displacement modes are the major factors involved in this study. Therefore, the magnitudes of the displacement distributions are used as the adaptivity indicator, considering the features of the surface acoustic waves that the displacements and potentials decay (to zero) away from the wave propagating surfaces.

In this paper it is found that the Lagrange finite element analysis method with a simple adaptive mesh generator is very powerful for evaluating how the metal electrodes affect the SAW propagating frequencies and velocities in the piezoelectric substrates on micro- and nano-meter scales. Numerical and application examples testify the finite element methods previously described in the last section of this paper.

VIBRATION AND SAW WAVE COMPUTATION AND ITS APPLICATION

The first test problem is a comparative study to verify the numerical convergence (rate) of generalized plain strain Lagrangian finite element methods (FEM) and plate FEM in bulk wave analysis. Let l, h and t be length, height and thickness respectively, then the test problem is a big quartz beam substrate ($l \times h \times b = 40m \times 2m \times 2m$) on macro-scale with free boundary conditions for computing the bulk wave frequency spectrum normalized by the fundamental thickness-shear frequency in Eq. (10b). For bulk wave analysis, two uniform meshes (adaptivity $r = 1.0$) are used for comparing the numerical convergence accuracies (Fig. 2).

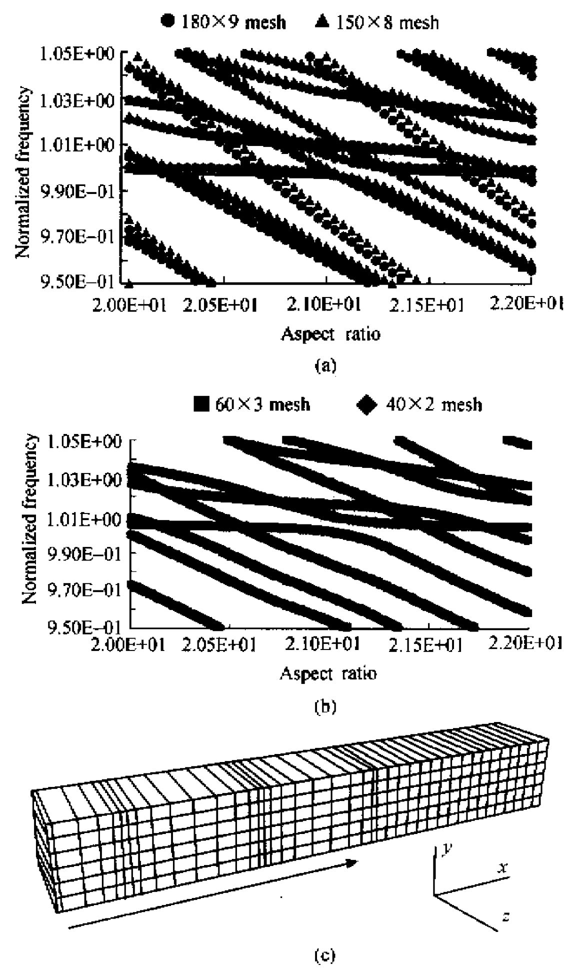

Fig. 2 (a) ST-cut BAW wave frequency spectrums in a vibrating plate by 3rd order mindlin plate FEM; (b) ST-cut BAW wave frequency spectrums in a vibrating solid using 3rd order lagrange generalized plain strain finite element method; (c) bulk acousticp-wave propagation in a solid

Some inconsistent results for AT-cut substrates based on high order piezoelectric plate theories were given and compared with experimental data by Wang, Yong and Imai, 1999. By solving a similar problem of ST-cut quartz substrates(Fig.1a), it is found that the plate element method is not accurate enough to be convergent for the case of piezoelectric analyses.

By proposing the high order Lagrange finite element methods in this paper, the FEM results in this paper converge well and fast with high accuracy(Fig.1b), the prescribed relative error of this bulk wave analysis can be very small and less than 0.002%.

Bulk acoustic waves(BAW) are a mixture of p-wave, and shear and bending waves. P-wave propagation is shown in Fig.2.

The second application problem is to analyze a practical SAW resonator with layered materials and interfaces between quartz substrate and aluminum electrodes(Fig.3). The quantitative relationship between them is to be computationally studied, as the accurate experimental results are hard to acquire for this case.

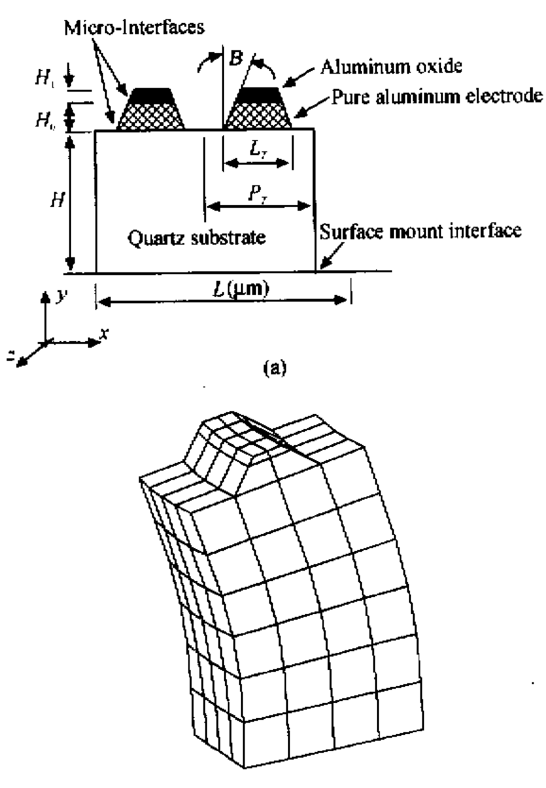

Fig.3 Amplified cross view of a periodical SAW resonator SMT structure with interfaces between surface mounted piezoelectric substrate, metal electrodes and aluminum oxide wear layers
(a) a period of resonator structure;
(b) deformed FEM mesh for half period

The finite element boundary conditions for half-wavelength (PT) analysis of SAW wave propagation in x direction have to be correctly enforced and are given as follows,

$$u_x^{\text{left}}(x = x_1) = u_x^{\text{right}}(x = x_1 + PT) = 0,$$
$$u, v, w, \phi \qquad (11)$$

The geometry and mesh of a periodical resonator structure are given in Fig.3 and Fig.4 respectively.

Fig.4 Half period adaptive lagrange finite element mesh for a tiny surface acoustic wave device with sloped metal electrodes

Fig.3(a) is a periodical part of a piezoelectric SAW resonator to be designed originally with micrometer dimensions. This resonator structure is reduced to nanometer scale for computational investigations here.

Fig.3(b) and Fig.5 show clearly similarities of piezoelectric and seismic surface wave propagations in SAW resonator structures and vibrating buildings in the earthquake.

Now with uniform meshing in the x direction of SAW propagation, the mesh enrichment or remeshing formula along the depth(y) direction is given and reviewed here by using a simple geometric progression:

$$dy_0 = 0$$
$$y_1 = y_1 + dy_0$$
$$y_2 = y_1 + dy_1$$
$$\cdots$$

where

$$dy_2 = (1 + r)dy_1$$
$$dy_3 = (1 + r + r^2)dy_1$$
$$\cdots$$

where the common ratio r is used as the local mesh enrichment indicator. When $r = 1.0$, the mesh is uniform. This simple mesh enrichment is found to be surprisingly effective and easy to use if appropriate finite element methods are selected for h-adaptive analysis of surface acoustic waves.

In Figs. 3 and 4, the electrodes will affect the SAW frequencies and velocities in the substrates and the FEA codes are very useful for analyzing the relationship between the SAW velocities and the geometric and material characteristics of the electrodes (Tables 1 and 2), which is an advantageous alternative over the analytical and experimental approaches for this resonator case.

Table 1 Computed nanometer scale lower and upper limit frequencies & SAW velocities in piezoelectric quartz substrate with metal electrodes

Wave length(nm)	No. of found eigenvalues	Substrate elements	Electrode elements	SAW mode displacements		
1.00000E+01	2	400	4			
SAW wave mode	Normlized frequency(Hz)	Actual frequency(GHz)	SAW wave velocity(m/s)	*u*	*v*	*w*
1	0.7550678E+01	0.311616E+03	0.311616E+04	28.6	69.9	1.5
2	0.7627985E+01	0.314806E+03	0.314806E+04	16.6	81.7	1.7

Table 2 Computed SAW velocities vs cut angle on nano-scaled free quartz substrate surface (prescribed relative error ≤ 0.04%)

Cut angle	16-node FEM	9- or 16-node FEM	Free surface/No electrodes	
	Computed	Computed	Exact (Datta, 1986)	Experimental (Zhang, 1998)
	Piezoelectric SAW velocity(m/s)	Mechanical SAW velocity(m/s)	Piezoelectric	Mechanical
90.00	3262.04	3261.46		
50.00	3173.11	3165.98		
33.00 (ST-cut)	3159.14#	3147.65# 3147.14*	3158.00	3149.70

* using a uniform mesh of 2000 nine-node Lagrange elements

\# using an adaptive mesh of sixteen-node Lagrange elements or a uniform mesh of sixteen-node elements

From Table 1, an interesting phenomenon is shown that when there are interfaces between substrates and electrodes interfering with the wave propagation, the SAW velocities will decrease and there are two SAW velocities of a stopband, rather than one standing-wave velocity in the case of no electrodes. The above accurate quantitative and qualitative relationship discovered by finite element computation is essential in actual micro resonator design in the future (Zhang, et al., 2002).

Both lower and upper limit velocities for St-cut angle tend to be 3158m/s as the electrode decreases in size and weight. The third benchmark test problem is to numerically compute the high frequency surface acoustic wave (SAW) velocity in a quartz crystal substrate without electrodes on the nanometer level, so as to compare the computed results with the exact solution; The studies for piezoelectric microstructures on the micrometer level were also carried out in a related paper. The results are given in Table 2 and Fig.5.

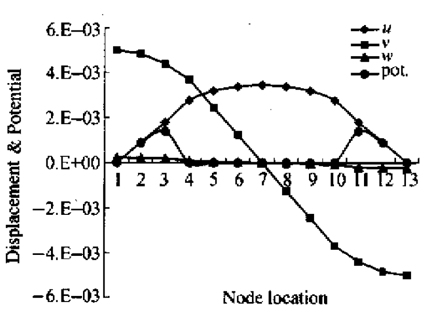

Fig.5 Piezoelectric finite element computed top displacements (u, v, w) and potential (amplified) of high-frequency surface acoustic wave propagation in a nano-scaled resonator structure with metalized electrodes

Table 2 shows that the adaptive 16-node FEM for piezoelectric and mechanical SAW wave analysis is accurate and much more efficient and 75% cost saving in the number of elements than the ordinary uniform meshing method.

The new computed SAW displacements and

potential on the nanometer level are described in Fig. 5. Check the p-wave and SAW displacement distributions on the Saw propagating surface in Figs. 5 and 2 with existing acoustic wave theories without electrodes, it can be seen the piezoelectric finite element computed results and methods in this paper are concrete and correct, and are providing a more convenient and accurate alternative than the costly high-resolution experimentation (Hesjedal and Chilla, 1997) for this case of high frequency data acquisition, and will be a new trend in solving the related cannot-see difficult problems in theory and practice.

CONCLUSIONS AND DISCUSSIONS

1. The proposed higher order adaptive Lagrangian generalized plain strain finite element methods and new computer programs are found to be very effective for the analysis of periodical SAW and BAW resonator structures, and very useful for discovering the relationship between the mechanical and electric fields.

2. It is essential to select the right computing methods for the accurate analysis of high frequency acoustic waves in a structure. It has been found in this paper that neither the lower order FEM and higher order plate element method is accurate enough, but the proposed higher order Lagrange finite element method is proved to be sufficiently accurate for GHz high-frequency acoustic waves in the structures with layered materials and nano-interfaces.

3. The discussed adaptive finite element approach has to be further modified for full-scale piezoelectric analysis of high frequency piezoelectric resonator structures, and new finite element program SAW9FEAP for piezoelectric and seismic SAW waves are developed for one-period of accurate wave analysis. However, because of the generality characteristics of finite element theories originally developed in civil and aerospace engineering, the developed finite element methods and computer programs with a special eigenvalue solver available have great potentials and can be applied and extended to solve related problems in dynamic vibrations and wave propagations in macro, micro and nano structural engineering respectively.

References

Datta, J., 1986. Surface Acoustic Wave Devices, Prentice – Hall, Englewood Cliffs, NJ

Desai, C. S., Zhang, W., 1998. Computational aspects of disturbed state constitutive models. *Computer Methods in Appl. Mech. Engrg.*, **151**: 361 – 376.

Hesjedal, T., Chilla, E., Fröhlich, H. J., et at., 1997. Surfing the SAW: Visualizing the oscillation of Au(111) surface atoms. Proc. IEEE Ultrasonics Symp., Toronto, Canada.

Hong, T., Teng, J. G., Luo, Y. F., 1999. Axisymmetric shells and plates on tensionless elastic foundations. *Int. J. Solids and Structures*, **36**: 5277 – 5300.

Hossack, J. A., Hayward, G., 1991. Finite – element analysis of 1 – 3 composite transducers. *IEEE Trans. Ultrason. Ferroelec. Freq. Controls*, **38**: 618 – 629.

Mindlin, R. D., 1955. An Introduction to the Mathematical Theory of Vibrations of Elastic Plates, US Army Signal Corps Eng. Lab., Fort Monmouth, New Jersey.

Mindlin, R. D., 1972. High frequency vibrations of piezoelectric crystal plates. *Int. J. Solids and Structures*, **8**: 895 – 906.

Mindlin, R. D., 1984. Frequencies of piezoelectrically forced vibrations of electroded quartz plates. *Int. J. Solids and Structures*, **20**(2): 141 – 157.

Steward, J. T., Chen, D. P., 1997. Finite element modeling of the effects of mounting stresses on the frequency temperature behavior of surface acoustic wave devices. Proc. IEEE Ultrasonics Symp., Toronto, Canada.

Wang, J., Yong, Y. K., Imai, T., 1999. Finite element analysis of the piezoelectric vibrations of quartz plate resonators with higher-order plate theory. *Int. J. Solids and Structures*, **36**: 2303 – 2319.

Yong, Y. K., Cho, Y., 1996. Numerical algorithms for solutions of large eigenvalue problems in piezoelectric resonators. *Int. J. Numerical Methods Eng.*, **39**: 909 – 922.

Zhang, W., 1993. Theoretical basis and general optimal formulations of isoparametric generalized hybrid/mixed finite element model for improved stress analysis. *Acta Mechanica Sinica*, **9**(3): 277 – 288.

Zhang, W., Chen, D. P., 1997. The path test conditions and some multivariable finite element Formulations. *Int. J. Numerical Methods Eng.*, **40**: 3015 – 3032.

Zhang, W., Yong, Y. K., Shigeo, Kanna, 1998. SAW16FEM program for high frequency micro piezoelectric SAW resonator analysis. Int. Joint Report, Seiko Epson and Dept. of Civil and Environ. Eng., Rutgers University, NJ.

Zhang, W., Tang, J. C., 2002. Constitutive computational modeling of piezoelectric microstructures and application to high-frequency SAW wave chip resonators. *Acta Mech. Sinica*, **18**: (in printing).