Study of PMN-PT Single Crystals for Resonator Applications

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***Abstract*—In this paper, the use of a lead magnesium niobate-lead titanate (PMN-PT) single crystal disk as a resonator has been explored. Finite Element Method (FEM) has been used to simulate both the impedance spectrum and vibration displacement for the PMN-PT disk. Because of the spurious modes, the disk with a full electrode or a partial electrode does not exhibit a clean resonance peak of the fundamental thickness mode vibration. However, a partial electrode can effectively confine the fundamental mode vibration in the electroded region, while the spurious mode vibration still spreads over the whole disk. By using an epoxy support along the edge, these spurious mode vibrations can be absorbed and a clean resonance response can be obtained. In addition to the excellent piezoelectric properties, the PMN-PT single crystal should be a promising material for resonator applications.**

I. INTRODUCTION

Lead magnesium niobate with 33 mol% of lead titanate (0.67PMN-0.33PT, abbreviated as PMN-PT), single crystals exhibit extraordinary large piezoelectric coefficient d_{33} (> 2000 pC/N) and electromechanical coupling coefficient k_{33} (> 90%) after being poled in [001] of the cubic coordinates [1-4]. They have attracted considerable attention and their use in various devices has been actively pursued. For comparison, the commonly used piezoelectric ceramic lead zirconate titanate (PZT-5H) has a d_{33} of ~ 600 pC/N and a k_{33} of ~ 0.75. The PMN-PT single crystals have been shown to provide better sensitivity and bandwidth than PZT when used in medical imaging transducers [5-6]. However, there is little work reported on the study of their use in resonator applications.

In use, it is necessary to support the piezoelectric resonators for the connection with peripheral electronics. They should be ideally supported at vibration nodes so as to minimize the resulting effects on the vibration and hence the overall characteristics. However, it is very difficult to support the resonators at points; and so they usually tend to experience fluctuation and degradation of device characteristics due to leakage of vibration energy. In order to realize piezoelectric resonators with low loss and high reliability, it is then of great need to confine vibration energy in a localized region and leave the supporting area free from vibration.

On the other hand, the impedance response of a piezoelectric resonator (with the electrode of the same size of the piezoelectric plate) usually exhibits numerous spurious vibrations adjacent to the primary vibration. These spurious vibrations, which are mainly the inharmonic overtone modes, result from the lateral propagation of elastic waves in plates and reflection from the boundaries and deteriorate the resonator characteristics considerably.

Electrode of smaller size than the piezoelectric plate is commonly used to minimize the influence of the mechanical support at the edges (leakage of vibration energy) and to suppress the spurious modes. For those resonators, the vibration of the desired resonance mode is confined or the corresponding vibration energy is trapped in the vicinity of the electroded region. This phenomenon is called energy-trapping and has been studied in detail [7-10]. Based on the wave theory and cutoff phenomenon for a lossless waveguide, general guidelines for determining the electrode dimension have been established. However, those guidelines are derived from simplified models (e.g. isotropic elasticity) on certain simple resonators (e.g. semi-infinite plate), so they provide only basic prediction and limited information of the resonance responses, in particular the vibration profile of the resonators. In this work, the finite element method will be used to study the resonance responses of the PMN-PT single crystals. The vibration profile as well as the impedance spectra will be modeled, from which the spurious response will be examined.

II. FEM MODELLING

In this study, a commercial finite-element code, ANSYS 9.0, was used to model the resonance responses of a PMN-PT single crystal disk. The disk has a diameter of 10 mm and a thickness of 1 mm, and is fully poled along the thickness direction (which is the [001] direction). Circular silver electrodes of diameter 10 mm or 2 mm and thickness 6 µm were applied on both the top and bottom surfaces and a lossy epoxy support was applied along the edge of the disk (Fig. 1). Both silver and epoxy are isotropic, whilst the poled

PMN-PT disk has a pseudotetragonal *4mm* symmetry (thus having 11 independent electroelastic constants: six elastic constant c, three piezoelectric constants e, and two dielectric constants ε). The material parameters (with conventional symbols) of each material used for the simulation are listed in Table I and II, respectively. It is assumed that the PMN-PT single crystal is lossless while the lossy epoxy has a damping factor of 10^{-5}. A 3-D 20-nodes brick coupled field element SOLID-226 was used to build up the model. Because of the symmetry, only a quarter of the circular disk was modeled and displacement symmetry boundary condition was applied to the interior areas. The PMN-PT disk was meshed in tetrahedral, while the silver electrodes were meshed in prism. A voltage of 0.5 V was applied to the top electrode and a voltage of 0 V was applied to the bottom electrode. Harmonic analysis was carried out to simulate the impedance spectra and vibration displacements.

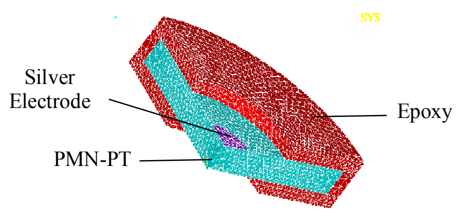

Figure 1. Figure 1 Schematic diagram of the PMN-PT single crystal disk used for the FEM analysis.

TABLE I. MATERIAL PARAMETERS OF PMN-PT SINGLE CRYST

c_{11}^E	c_{12}^E	c_{13}^E	c_{33}^E	c_{44}^E	c_{66}^E
115 GPa	103 GPa	102 GPa	103 GPa	69 GPa	66 GPa
e_{15}	e_{31}	e_{33}	ε_{11}^S	ε_{33}^S	ρ
10.1 C/m^2	-3.9 C/m^2	20.3 C/m^2	1434	680	8060 kg/m^3

TABLE II. MATERIAL PARAMETERS OF SILVER AND EPOXY

	Silver	Epoxy
Elastic Modulus (GPa)	72.4	2
Poisson's Ratio	0.37	0.4
Damping Factor	0	10^{-5}
Density (kg/m^3)	10500	1

III. RESULTS AND DISCUSSION

To illustrate the resulting effects of energy-trapping, the impedance spectrum of a PMN-PT disk with a full electrode (i.e. diameter = 10 mm) was first examined and the simulated results are shown in Figure 2. It can be seen that the main resonance peak which is associated with the fundamental thickness mode is not clean and coupled or interfered significantly by a number of spurious modes which are most likely the inharmonic overtone modes of the thickness-mode vibration. For a circulate resonator with clamped boundaries both at the surfaces and edges, the resonance frequencies are given by [9]:

$$f_{nmk} = \frac{v}{2\pi}\sqrt{\frac{n^2\pi^2}{t^2}+\frac{\chi_{mk}^2}{a^2}} \qquad \begin{array}{l} n = 1,3,5,.. \\ m = 0,1,2,3,.. \\ k = 1,2,3,... \end{array} \qquad (1)$$

where v is the wave velocity, t and a are the thickness and radius of the resonator, χ_{mk} is the kth root of Bessel's function of order m. The calculation shows that, for the PMN-PT disk, the inharmonic overtone resonance modes are very close to the fundamental resonance mode (f_{101}), e.g. f_{111} - f_{101} ~ 50 kHz. Because of coupling, the vibration at the resonance frequencies becomes interfered, resulting in the degradation of the resonator performance. Figure 3 shows the displacement profile at 1.86 MHz. It can be seen that there are ripples superimposed the fundamental-mode displacement over the whole disk. It should be noted that the PMN-PT single crystal is assumed to be lossless, so the observed spurious modes from the simulation may be stronger than those for the real sample. However, it is still worth to make the assumption as the effects of the epoxy support can be clearly demonstrated (which will be discussed below).

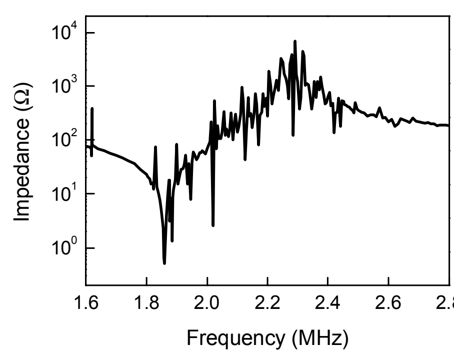

Figure 2. Simulated impedance spectrum for the PMN-PT single crystal disk with a full electrode.

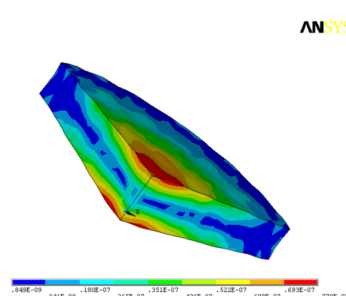

Figure 3. Simulated displacement profile at 1.86 MHz for the PMN-PT single crystal disk with a full electrode.

Figure 4 shows the simulated impedance spectrum for a PMN-PT disk with a partial electrode (diameter = 2 mm).

The main resonance peak is still interfered significantly by the spurious modes. It is also noted that the resonance peak becomes narrower with f_s (the frequency at which the first impedance minimum occurs) shifted towards higher frequencies, from 1.86 MHz to 1.91 MHz. This suggests that as the electrode decreases, the vibration is confined in a smaller region [referring to (1)]. This is in agreement with the displacement profile simulated at 1.91 MHz (Fig. 5). It has been noted that at higher frequencies, the vibration becomes spreading over the whole disk. As there is no epoxy support, these vibrations in the un-electroded region will not be absorbed, thus resulting in the interference of the fundamental vibration.

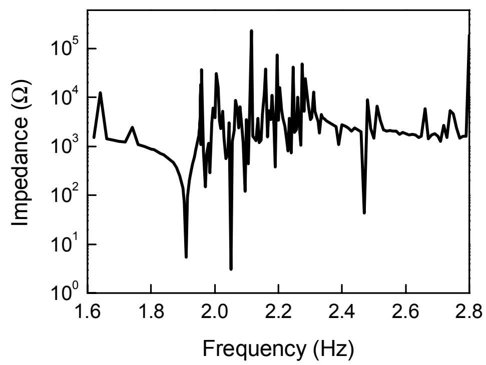

Figure 4. Simulated impedance spectrum for the PMN-PT single crystal disk with a electrode of diameter 2 mm.

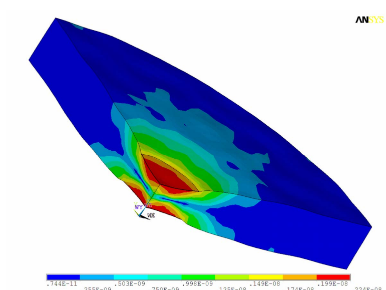

Figure 5. Simulated displacement profile at 1.91 MHz for the PMN-PT single crystal disk with a electrode of diameter 2 mm.

Figure 6 shows the simulated spectrum of a PMN-PT disk with a partial electrode (diameter = 2 mm) and an epoxy support of width 3 mm along the edge. It can be seen that the impedance spectrum becomes clean, with only a slight interference at high frequencies. This should be attributed to the absorption of all the spurious mode vibrations in the un-electroded region by the lossy epoxy support. As the fundamental mode vibration is mainly confined in the electroded region, it is not affected significantly. Figures 7 and 8 show, for example, the displacement profile simulated at f = 1.96 MHz and 2.00 MHz, respectively. It can be seen that the disk vibrates mainly in the fundamental thickness mode, without significant interference, in the whole resonance region.

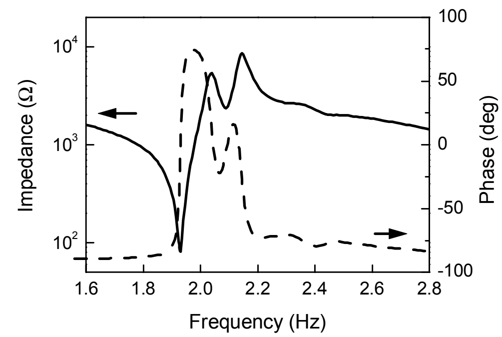

Figure 6. Simulated impedance spectrum for the PMN-PT single crystal disk with a electrode of diameter 2 mm and an epoxy support along the edge.

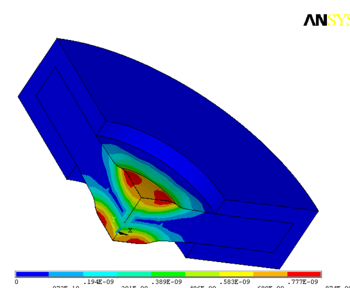

Figure 7. Simulated displacement profile at 1.96 MHz for the PMN-PT single crystal disk with a electrode of diameter 2 mm and an epoxy suport along the edge.

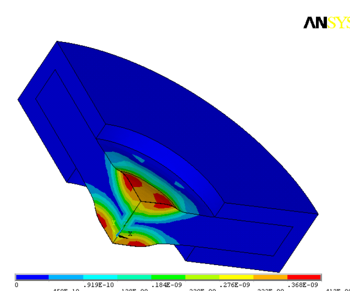

Figure 8. Simulated displacement profile at 2.00 MHz for the PMN-PT single crystal disk with a electrode of diameter 2 mm and an epoxy suport along the edge..

IV. CONCLUSION

Finite Element Method (FEM) has been used to simulate both the impedance spectrum and vibration displacement for a PMN-PT single crystal disk. Because of the spurious modes, the PMN-PT disk with a full electrode or an electrode of smaller diameter does not exhibit a clean resonance peak of the fundamental thickness mode vibration. The vibration displacement near the thickness mode resonance frequency in fact includes both the thickness mode vibration and other vibrations, such as radial mode vibrations. However, the thickness mode vibration is still dominant. A partial electrode can effectively confine the fundamental mode vibration in the electroded region, while the spurious mode vibration still spreads over the whole disk. An epoxy support along the edge can damp the spurious mode vibrations and give a clean resonance response. Accordingly, the PMN-PT single crystal should be a promising material for resonator applications.

ACKNOWLEDGMENT

This work was supported by the Innovation and Technology Fund (ITF UIT/071) of the HKSAR Government and Hong Kong X'tals Ltd., and the Center for Smart Materials of the Hong Kong Polytechnic University.

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