1983

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EFFECT OF MESA-SHAPING ON SPURIOUS MODES IN ZnO/Si
BULK-WAVE COMPOSITE RESONATORS

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Abstract

Bulk-wave composite resonators (BWCRs) employing thin piezoelectric films on silicon membranes have received considerable attention because of potential for integrated selectivity at VHF and UHF. The TE-mode zinc oxide on silicon configuration has received the most attention. A major design problem is the presence of close-in spurious modes on both low and high frequency sides of the fundamental. Mesa-shaping of the BWCR by etching the zinc oxide film in the region surrounding the top electrode has been shown experimentally to reduce the spuri, although this improvement has not been adequately explained. Here we describe further developments to a two-dimensional model which now includes acoustic loss into the membrane, and which predicts admittance at all frequencies, contrasting with earlier models which find solutions only at the resonant frequencies. This model is compared to experiment and is shown to explain the effect of mesa-shaping. Computer simulations illustrate the relationship between geometry and performance.

Introduction

Thin-film bulk-wave composite resonators (BWCRs) promise acoustic wave components which are compatible with ICs in terms of both size and technology1,2,3. BWCRs are fabricated by depositing thin films of zinc oxide (or other piezoelectric material) onto a silicon membrane of the order of a few microns thickness, with electrodes on both surfaces of the piezoelectric film. This configuration is shown in Fig. 1(a). The thin membrane area is supported by the surrounding bulk silicon, so the structure is robust. Both C-axis normal films for exciting thickness extensional (E) modes1,2 and inclined C-axis films for thickness shear (TS)3 modes have been studied. One application of BWCRs is for integrated filters at VHF or UHF. For maximum bandwidth high coupling coefficient is needed and the former type is therefore preferable. Simpler technology is another advantage of the TE mode configuration.

Filter specifications generally require high Q-factor and low level of spurious responses. Achieving high Q-factor is essentially a problem of technology while the spurious mode content is one of design. One method shown to be effective for reducing spurious modes is that of shaping the resonator in the form of a mesa2 as shown in Fig. 1(b). However the improvement has not been adequately explained. The shaping entails removal of the piezoelectric film from the area outside that of the top electrode. Extensions to a two-dimensional theory which now models both configurations in Fig. 1 are described here, and the predictions are compared to measurement and one-dimensional theory. An important new feature of the theory is that it is valid at all frequencies, and not just the resonances. In this respect the theory also differs from other multi-dimensional models5,6. The modification is shown to be necessary for describing the mesa-shaped device. The theory gives good agreement for the spurious mode content and also for the effect of mesa-shaping on these modes. Detailed field plots show why the method is effective. In addition experiment shows that other spurious modes are caused by the bond-pad. Further predictions are then made leading to optimum resonator designs.

Two-dimensional theory

Ref. 4 reported a two-dimensional model for finding the short-circuit modes of the BWCR. Here we describe extensions which make the theory more general in three respects: (a) the solution for
The solution is:

\[ u_2(0) = \frac{2}{\pi} \sum_{n=1}^{\infty} B_n \exp(-jk_n x_2) \]

\( \phi(0) = u_4(0) = \sum_{n=1}^{2} \frac{B_n}{n^2} \exp(-jk_n x_2) \)

\( u_2 = \frac{6}{n^5} \sum_{n=5}^{\infty} B_n \exp(-jk_n x_2) \)

For this a voltage of \( V \exp(j\omega t) \) is assumed to be applied between the electrodes, (b) propagating Lamb modes are included in the free-surface regions surrounding the top electrode and these are assumed to be absorbed into the bulk silicon rather than reflected at the membrane edges, and (c) the theory is applicable to the mesa-shaped as well as the constant-thickness configuration. The more complex geometry of the former requires more Lamb modes than in ref. 4 in order to satisfy the boundary conditions.

The solution is summarised in Fig. 2. The differential equations and the majority of boundary conditions are as described in Ref. 4. The additional boundary conditions are:

\[ \phi = 0 \text{ at } x_2 = b, \quad \frac{\partial u}{\partial x_3} = 0 \text{ at } x_2 = 0 \quad (1) \]

\[ T_{13} = 0 \text{ at } x_3 = \pm W/2, \quad c < x_3 < \beta \quad (2) \]

\[ u_1, \frac{\partial u_1}{\partial x_3} \text{ are continuous at } x_3 = \pm W/2, \quad -d < x_3 < c \quad (3) \]

where \( \phi \) is potential (written as \( u_4 \) for convenience), \( u_i = [i=2,3] \) is displacement and \( T_{ij} \) is stress. The boundary conditions at the membrane edge are dropped, with the membrane assumed to be of infinite extent in \( x_3 \) and \( j \) and the values 2 and 3 in equations (2) and (3).

The solution for particle displacement and potential is the sum of a one-dimensional field \( u_i(0)(x_3) \) \( i=2,3 \) confined to the region \( x_3 < W/2 \) and a Lamb mode series in each of the three regions \( x_3 < W/2, \quad x_3 = W/2 \) and \( x_3 > W/2 \). Each term in these series is the product of an unknown amplitude \( B_i \) and a function \( u_i(p)(x_3) \), \( i=2,3 \) found using the analysis of ref. 4. Displacement patterns for the lowest 9 modes (whether in the electroded or one of the free-surface regions) are shown schematically in Fig. 3. The additional field \( u_i(0) \) is required in the electroded region to satisfy equation (1) which clearly cannot be satisfied by the Lamb modes, for which the potential on both electrodes is zero. It is readily shown that, at arbitrary frequency \( \omega \), the one-dimensional admittance is obtained at arbitrary frequency \( \omega \).

It will be shown later that equations (4) to (6) give a fairly accurate solution for the fundamental mode. However the principal reason for deriving this field is to obtain a forcing term in the two-dimensional solution. The boundary conditions at the electrode edges (equations 2 and 3) are approximated by performing Fourier analyses of \( T_{13} \) over the interval \( -d < x_3 < c \) and of \( u_1 \) over \(-d < x_3 < c \). Truncating these Fourier series then gives a finite set of boundary conditions which on substitution of...
the solutions for \( u \) (and corresponding stress fields \( \sigma \)) shown in Fig. 2 gives a set of linear equations which are solved for the amplitudes \( D \). Clearly the number of Lamb modes must match the number of terms in the truncated Fourier series. It is typically found that, for the mesa-shaped resonator, the boundary conditions are accurately satisfied if we take the lowest 5 Lamb modes in each of the free-surface regions (making sure that the sign of the wavenumber is such that each mode is evanescent or propagating away from the electrode), and the lowest 9 Lamb modes in the electroded region (18 counting both positive and negative wavenumbers). These are then used to satisfy the boundary conditions on the 0th and 1st spatial harmonics of \( T_{22} \) and \( T_{33} \) in equation (2), the 0th, 1st and 2nd harmonic of \( u_3 \) and \( \partial u_3/\partial x_3 \), and the 0th and 1st harmonic of \( u_2 \) and \( \partial u_2/\partial x_3 \) in equation (3). With this choice, and taking the boundary conditions at both \( x_3 = -W/2 \) and \( x_3 = +W/2 \), the number of complex equations is 28. This is equal to the number of unknowns \( D \). The dispersion of the Lamb modes for one value of material thickness ratio are shown in Fig. 4. For the constant thickness resonator the boundary conditions on \( T_{22} \) are dropped and only the lowest 5 Lamb modes in the electroded region are required.

Having obtained the full solution for the electrical and mechanical fields, it remains to integrate the normal electric flux density \( D \) over the electrodes to obtain the charge on the electrodes, differentiate with respect to time to obtain the current \( I \), and divide this by \( V \) to give the admittance of the resonator.

Comparison between theory and experiment

A small number of resonators have been made with zinc oxide deposited by the Murata Manufacturing Company. Their performance is compared here with the above theory. The most useful parameter for comparison is susceptance since this shows both electrostatic and acoustic contributions to the response. A typical curve measured on a network analyser is shown in Fig. 5(top). The resonator dimensions were: \( d = 7.0 \, \mu m \), \( b = 9.7 \, \mu m \), \( W = 0.5 \, mm \). The main resonance is at \( 224 \, MHz \) and has a Q of \( = 600 \). The spurious modes can be divided into three groups: (i) closely-spaced low Q modes \( = 10\% \) below the fundamental, (ii) higher Q modes just above the fundamental, and (iii) very few Q modes spaced at \( = 8 \, MHz \) intervals. This third group are harmonics of the transducer formed by bond-pad, zinc oxide film and bulk silicon. This phenomenon was referred to in refs 1 and 7, and was demonstrated here by bonding to the connecting strip and cutting the link to the bond-pad with a laser. The susceptance then measured and the computed response are shown in the centre and bottom diagrams of Fig. 5 respectively. There is a small frequency discrepancy due to uncertainty in the thickness and the general susceptance level is higher than predicted due to stray capacitance. Most of the extra static capacitance vanished when the bond-pad was excluded, but a contribution from package and bond-wires remains. Q-factor is generally lower than predicted due to imperfections in the membrane and exclusion of parasitic resistance\(^7\) in the theory. The 1-D model (broken curve) predicts only a loss-less fundamental mode whereas many of the spurious modes are predicted by the 2-D model. Both the group of low-Q modes some 10\% below the fundamental and the group of high-Q modes on the high frequency side are predicted. However in practice there are more modes in both groups, suggesting that a full 3-D theory may be required. Nevertheless the 2-D model gives good qualitative agreement. Detailed field plots of one of the low-Q modes and the three high-Q modes are shown in Fig. 6. Components of motion in phase and quadrature with the applied voltage are illustrated, the latter representing the motion a quarter of cycle earlier. The low-Q modes are essentially TS2 vibrations with most of the energy leaking away through the membrane. (The waves appear to travel towards the electrode, but of course power flows in the opposite direction. This unusual effect arises because of the negative dispersion of the TS2 mode for this geometry). The high-Q modes are the fundamental, third and fifth inharmonic TE1 modes which are clearly trapped in the electrode.
The enlarged views of the vibration at one electrode edge show in all cases that the field matching is excellent.

The effect of mesa-shaping is now considered. The susceptances before and after removal of the zinc oxide film, and then excluding the bond-pad as before, are shown in Fig. 7 together with the prediction. Shaping is seen to reduce the Q-factors of the spurious modes without significantly affecting the fundamental. The effect of removing the bond-pad is to eliminate the very low Q modes as before. The Q-factors of the improved device are ≤1000 at both series and parallel resonant frequencies. The 2-D model again agrees qualitatively with experiment. The better suppression predicted is discussed below. Fig. 8 shows the vibration at the fundamental and spurious mode frequencies. It is clear that energy-trapping no longer occurs. Substantial mode conversion takes place at the electrode edges. Much of the energy is converted to the E1 and E2 modes which propagate away through the membrane into the bulk silicon resulting in very low Q-factors. In practice however, some energy is reflected back from the membrane edge accounting for the higher measured Q. The application of absorbent material to the surface outside the electrode is expected to improve the suppression and give better agreement with the theory. The fundamental mode which is still strongly excited is not really a mode, but is essentially the one-dimensional driving field \( u_0(x) \). There is substantial stored energy in this field, as shown in Fig. 8(a) by the large in-phase component of strain which is independent of \( x_3 \). This results in a high predicted Q-factor despite the leakage into propagating modes. Strictly the mesa-shaped device is more like a transducer in terms of its mechanical behaviour, since there are no high-Q short circuit modes. However its electrical performance is that of a single mode resonator with a theoretical upper
measured including bond-pad

Fig. 7 Measured susceptance before and after mesa-shaping, with and without the bond-pad, and predicted susceptance of mesa-shaped BWCR.

Optimum Geometry BWCRs
The level of agreement between theory and experiment suggests that the model can be used with some confidence to optimize resonator design. The major application being considered at present is in wideband filters (up to 5%). High ratio of motional capacitance $C_m$ of the fundamental mode to static capacitance $C_s$ is therefore required. The 1-D model is adequate for finding this ratio and also the capacitance ratios $C_m/C_s$ of the "harmonic" overtone TE modes (n=2,3,...), the nth mode being that for which there are approximately n half wavelengths of extensional motion in the total composite thickness. Fig. 9 shows that a ratio of silicon to total thickness of 0.25 gives the best compromise between coupling to the fundamental and rejection of higher overtones. This result is essentially independent of electrode width.

The 2-D model is now used to predict the effect of keeping the thickness ratio at 0.25, but changing the normalised electrode width $W/a$. The susceptances for constant thickness BWCRs with five different values of $W/a$ are shown in Fig.10. These suggest that $W/a$ should be <9. Below this value only the fundamental mode is energy-trapped, although the weakly coupled modes some 10%, below the fundamental frequency still appear. For higher values of $W/a$ inharmonic modes become trapped. However small electrode area implies high impedance which may lead to problems in filter design. In such situations it would be appropriate to use the mesa-shaping for spurious mode suppression. Fig.11 shows the predicted susceptances for the same values of $W/a$ with all the zinc oxide removed from the free-surface region. Comparison with Fig.10 shows that for wider electrodes ($W/a = 20$ and $30$) there is improvement in performance, but for narrower electrodes spurious levels are increased.

Conclusions
Mesa-shaping has been shown to be effective for reducing the Q-factor of spurious modes in TE mode BWCRs. Computer simulations of the electromechanical field show that conventional energy-trapping is prevented by mode conversion at the step discontinuity, and also suggest that an independent of electrode width.

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absorber would increase the effectiveness of the shaping. Other spurious modes can be eliminated by ensuring that the bond-pad connected to the top electrode does not overlap the bottom electrode. A two-dimensional model has been developed for predicting the admittance at arbitrary frequency, and this shows good qualitative agreement for the spurious modes and the effect of the mesa-shaping. The fundamental mode is shown to retain its high Q-factor through the stored electrical and mechanical energy directly coupled to the applied field. Further predictions show that, for BWCRs with maximum coupling coefficient, mesa-shaping would improve low impedance resonators but degrade those with high impedance.

The authors gratefully acknowledge the contribution of Mr S Fujishima and colleagues at Murata Manufacturing Co. Ltd. who provided the zinc oxide films.

This work was carried out with the support of Procurement Executive, UK, Ministry of Defence, sponsored by DCVD.

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