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Assessment of the shear acoustic velocities in the different materials composing a high frequency solidly mounted resonator

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ABSTRACT

Thin film acoustic resonators operating in the shear mode are being increasingly used for in-liquid sensing applications. A good design of such sensors requires accurate knowledge of the acoustic properties of the materials composing the whole device, which specifically includes their shear velocities. Here we present a method to assess the shear acoustic velocity of high and low acoustic impedance films commonly used in AlN-based solidly mounted resonators (SMRs), using test devices specifically designed to induce a half-wavelength resonance in the layer under study. Provided that the thickness and mass densities of all the layers are known, fitting the electrical response by Mason's model over a wide frequency range gives accurate values of both longitudinal and shear mode velocities. The assessment of porous and dense SiO_2, Mo, W and Ta_2O_5 sputtered films yields shear velocities of 3150 m/s, 3950 m/s, 3450 m/s, 3350 m/s and 2900 m/s, respectively. In addition, the resonances stimulated in the Ir and Au top electrodes enable deriving their shear modes velocities, with values of 3950 m/s and 2350 m/s, respectively.

1. Introduction

Quartz crystal microbalances (QCM) operating in liquid media have demonstrated the potential of shear acoustic wave resonators in the area of gravimetric sensors [1]. Since their relative sensitivity increases with frequency, resonators operating at GHz frequencies are expected to push down detection limits, as already stated in the late fifties [2]. High frequency resonators make use of piezoelectric thin films, which also offers the possibility of integrating them in a multisensory chip. For these reasons, bulk acoustic wave (BAW) resonators based on AlN or ZnO films are being developed as an alternative to QCMs for bio-chemical applications [3,4]. For in-liquid operation, BAW resonators operating in shear modes are preferred because the movement of the material parallel to the surface is not hampered by the surrounding liquid. This overcomes the attenuation suffered by longitudinal modes forced to displace the adjacent fluid in their movement normal to the surface, which results in an increase of their quality factor *Q*.

Two different ways to excite shear modes in ZnO and AlN films have been reported. The most straightforward, known as lateral excitation, consists in applying an electric field parallel to the surface of a c axis oriented through two coplanar electrodes, to excite the shear wave by virtue of the d_{15} piezoelectric coefficient [5]. In practice, lateral excitation provides extremely weak electric fields between the electrodes and, hence, hardly noticeable shear excitations [6,7]. Alternatively, shear modes are effectively generated by normal excitation of films exhibiting the *c*-axis tilted with respect to the surface normal, through the component of the electric field perpendicular to the *c* axis and the d_{15} coefficient. Although AlN and ZnO films tend to grow with the *c*-axis normal to the substrate, films with tilted grains can be achieved by sputtering on roughness-controlled substrates displaced from the center of the target which encourages the growth of the microcrystal along the direction of the impinging species [8]. Well-performing resonators require acoustic isolation to avoid energy losses through the substrate that reduce their Q, which is commonly achieved by two methods. The first consists in producing an air gap between the resonator and the substrate so that energy losses can only take place through the supports because the acoustic radiation to the air is minimal. These structures, called free-standing film bulk acoustic resonators (FBAR), require complex fabrication technology and exhibit too high a thermal isolation that limits power handling. The alternative method is the use of acoustic reflectors between the resonators and the substrate, giving rise to the so-called solidly mounted resonators (SMR) [9]. Bragg mirrors are typical acoustic reflectors formed by alternating quarter-wavelength-thick layers ($\lambda/4$-layers) with low and high acoustic impedance [10]. The achieved acoustic isolation (reflection coefficient) increases with

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the number of layers and with the mismatch between the acoustic impedances of two consecutive layers.

For a proper design of SMRs, the properties of all their constituents (piezoelectric, electrodes and acoustic reflector) must be accurately known, since their acoustic impedance (product of the mass density and acoustic velocity) is essential for the isolation of the acoustic waves. However, whereas the longitudinal velocities of the materials commonly used in SMRs are well known, few data on the shear velocities at the typical GHz frequencies have been reported; these are frequently taken as half the longitudinal velocity for practical purposes [11]. Moreover, films grown by different techniques exhibit significantly different properties, which requires specific characterization.

In this paper we propose a procedure to assess the shear mode properties (mass density, sound velocity and acoustic impedance) of typical thin film materials commonly used as low or high acoustic impedance material for acoustic reflectors (porous and dense SiO_2, Mo, W and Ta_2O_5). The characterization is performed through the analysis of all the resonances (shear and longitudinal) excited in specific test resonators using containing asymmetric reflectors operating at GHz frequencies.

2. Design of the structure and method of analysis

The method proposed for measuring the sound velocity of the layers composing SMRs was previously developed for assessing the longitudinal modes [12–14]. Briefly, it consists on significantly increasing, in the acoustic mirror, the thickness of the layer under study that is closer to the piezoelectric stack. When exciting the whole device, in addition to the fundamental resonance, a $\lambda/2$ resonance is induced in the thickened layer. By fitting the electrical response of the resonator over a wide frequency range through Mason's model, one can deduce the values of the sound velocity, which is taken as a variable. An essential requirement is that thickness of the layer under study is adjusted so that the corresponding $\lambda/2$ resonance appears in the band of the reflector, near the fundamental piezoelectric resonance.

The assessment of the shear velocities of the reflector layers using the method described below is significantly more complex. First, shear modes have to be excited, which requires growing AlN films with tilted microcrystals. Second, under normal excitation, both longitudinal and shear modes are excited, so one has to design acoustic reflectors that provide simultaneously large reflectance for both fundamental modes (longitudinal and shear) and for the $\lambda/2$ resonance induced in the layer under study. Third, the uppermost layers of the acoustic reflectors need thickening, in order to shift the induced $\lambda/2$ resonance to the bandwidth of the mirror, which considerably distorts the transmittance of the reflector. To highlight these effects, Fig. 1 displays the simulated impedance spectra of two resonators formed by piezoelectric stacks vibrating on top of reflectors made of $\lambda/4$ layers (called hereafter symmetric reflectors), and reflectors with an uppermost layer well above $\lambda/4$ (asymmetric reflectors). The transmittance of the mirrors for both longitudinal and shear modes is also shown.

Fig. 1 shows that thickening the uppermost layer of the reflector distorts its transmittance, which originates extra peaks in the electrical spectrum different from resonances and associated to the reduction of the acoustic reflectance at some frequencies. Test devices need careful designing to enable a precise identification of the resonances of interest, which usually requires designing identical devices with test layers of different thickness to obtain redundant results. Mason's model [5] allows fitting the spectra with the required precision whenever the materials constants and geometric dimensions are accurately known.

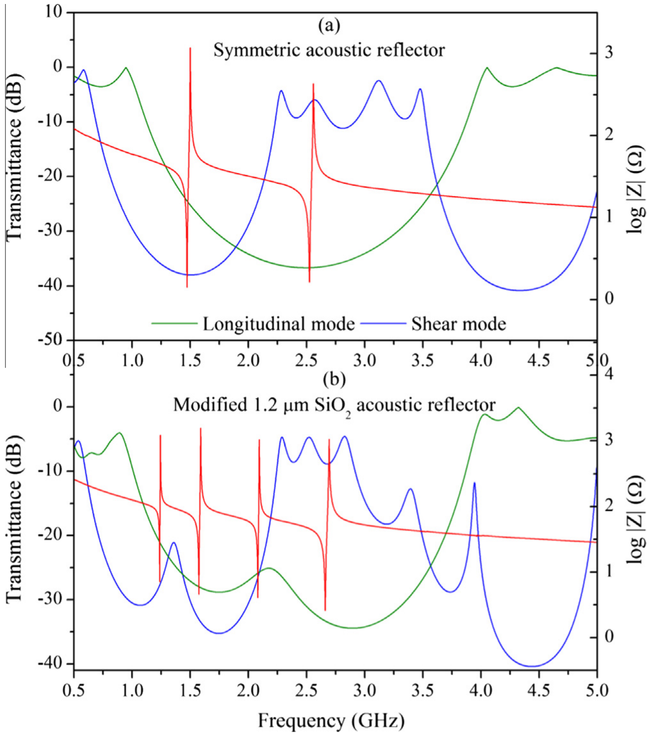

Fig. 1. Simulated frequency responses (red line) of two AlN-based SMRs tuned at 2.5 GHz (longitudinal mode) and containing a) a symmetric reflector alternating five $\lambda/4$ layers of SiO_2 and Mo, and b) an asymmetric reflector alternating four $\lambda/4$ layers of SiO_2 and Mo and terminated with a 1200 nm-thick SiO_2 layer. The figure also displays the simulated transmittance of the reflectors for the longitudinal modes (green line) and the shear modes (blue line). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Two sets of test devices (see Fig. 2) are proposed to assess the shear acoustic velocities of the low and high acoustic impedance layers composing the reflector. Both contain an identical piezoelectric stack and an asymmetric acoustic reflector with the layer under study closer to the stack considerably thickened.

After measuring the frequency response of the two test structures, an iterative method is used to derive the values of the shear velocities. The frequency response of the test device (a) is fitted in first place using Mason's model by setting initial values for the shear velocities of the electrodes (Ir and Mo) that can be refined afterward. This provides a first value for the shear velocity of the low impedance layer, which is used to fit the response of the test device (b) to derive a first value of the shear velocity of the high impedance layer. After a couple of iterations, the values of the shear velocities converge. Other materials, including new metallic electrodes, can be assessed afterward by following the same scheme and using new structures containing materials with properties already known.

3. Experimental

The test devices consisted of a piezoelectric stack formed by a 120 nm-thick Ir bottom electrode, a 1.1 μm-thick AlN piezoelectric layer and a 150 nm-thick Mo top electrode built on top of the acoustic reflectors. Si wafers were used as substrates. AlN films were sputtered in an ultra-high-vacuum system pumped to a base pressure below 1.3×10^{-6} Pa. A high purity aluminium target 150 mm in diameter was sputtered in Ar/N_2 atmospheres (40:60) using a pulsed-DC source (MKS ENI RPG-50E) operating at 250 kHz. Before the film deposition, an AlN seed layer was

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