Program for Calculating SAW Velocity on Piezoelectric Substrates with Finite Films Version 2.0

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1 Outline

This computer program calculates the complex velocities and electromechanical coupling factor K^2 of Rayleigh and/or Leaky-SAWs on piezoelectric substrates by the use of the effective permittivity theory. Provided that initial values required for the velocity search are adequate, all of physically proper and piezoelectrically excitable SAWs can be found without specifying their types. Effects of layers with finite thickness can be taken into account. Supported substrate materials are $LiNbO_3$, $LiTaO_3$, $Li_2B_4O_7$, GaAs, quartz, $La_3Ga_5SiO_{14}$ and $KNbO_3$ with Al, Au or SiO_2 as the film. Other substrates and/or films can be analysed by slightly modifying the source code. Note that K^2 is determined from the residue of the SAW poles appeared in the effective permittivity. This estimation is physically proper than that estimated by $2\Delta V/V$, which may cause large error when the SAW and bulk wave velocities are in close proximity.

As a new function embedded from the version 2.0, the program can output field distribution in the structure, and the output can also be used as an input data for making animation.

2 Usage

Type "VCAL" for execution.

1. "Enter File Name" where the output data will be stored. Note that, if the file already exists, the file will be overwritten and the former data will be erased.

2. "Enter 1-11 for LNOW(arner), LNON(akagawa), LNOK(ovacs), LTOW(arner), LTOS(mith), LTOK(ovacs), LBO, GaAs, quartz, LGS and KNO" for specifying the substrate materials. If you enter other value, the program will be terminated.

3. "Enter Axis & Angle" for specifying the rotation of the substrate and "To proceed next step, enter 0 for axis". For example, if desired substrate cut and SAW propagation direction is specified by the Euler angles $(45, 30, -20)$ in degree, type

   3,45 <CR>
   1,30 <CR>
   3,-20 <CR>
   0,0 <CR>

   Then the program prints the bulk wave velocities whose wavenumbers are parallel to the surface. If the piezoelectricity is decoupled with some displacement components u_i, the program displays its situation and does not display corresponding bulk wave velocities.

4. " Enter 1 for Al, 2 for Au or 3 for SiO_2" to specify the film material. Then the program prints the longitudinal and shear bulk wave velocities in the film.

5. "Enter hs/lambda" where h_s and λ are the metal thickness and SAW wavelength, respectively, "and icond" for specifying the surface electrical boundary condition, that is, 0 for open or 1 for short.

6. "Enter vs, ve and vint" where V_s, V_e, and V_{int} are the start, end and interval, respectively, of velocities for searching initial values of the SAW velocity manually. After typing, the program tabulates velocities and calculated determinants (complex value). The velocity giving zero determinant corresponds to the SAW velocity for specified h_s. Location of the solution can be found easily by searching velocity where the sign of real and/or imaginary parts of the determinant change. Once the zero of the determinant is estimated to within an accuracy adequate for an initial guess, "0 0 0" must be entered to proceed to the next step.

7. "Enter hs, he, hint and vstart" where h_s, h_e, h_{int} are the start, end and interval, respectively, of relative thicknesses where the SAW properties are to be estimated. V_{start} is the approximate value of the SAW velocity for $h = h_s$, and is estimated in the previous step. After typing, the program tabulates the relative film thickness, determined velocity V (m/sec), attenuation α (dB/λ), electromechanical coupling factor K^2, the effective permittivity $\epsilon(\infty)/\epsilon_0$, $\epsilon(0)/\epsilon_0$ and the absolute value of the determinant. These values are displayed and stored simultaneously into the file specified in the first step. Preceding the tabulated data, the specified values are also listed. When all of the iteration complete, the program reexecutes this step. For returning to step 2, enter "0 0 0 0".

2.1 Note

1. In the case of metal films, the free surface boundary condition is corresponds to set (1) the film conductivity as zero and (2) the film permittivity as ϵ_0.

2. When V_{start} is far from the exact value, the program may fail to find a solution, and will return to the previous step. This situation may occur when (1) the SAW velocity is too close to the bulk wave velocity, (2) the piezoelectric coupling for the SAW is too small or (3) h_{int} is too large.

3. When multiple SAW velocities are in close proximity, the program tends to find the solution with larger electromechanical coupling. So as to find the other one, one must determine more accurate SAW velocity in Step 6 for the use in Step 7.

4. In the software, the temperature is assumed to be 25°C. It can be adjusted by specifying the parameter "temp" in the main routines in "vcal.f".

3 Field distribution

Data format

At the step 7, if $h_{int} = 0$ is specified, field distribution in the substrate is calculated for $f = f_{start}$ and will be printed into the file "@up". The data format is,

X_3, u_1, u_2, u_3 and $10^{-10}\phi$

where u_i and ϕ are complex values.

3.1 Displaying instantaneous field distribution by GNUPLOT

The output can be used directly to display the instantaneous field distribution by using the free software "GNUPLOT". For example, ϕ can be displayed by,

```
gnuplot> set data style lines
gnuplot> splot "@up" using 1:8, "@ue" using 1:9
```

If you do not have the software, you can get through most of all anonymous ftp server. Note the software workds both UNIX and Windows environments.

3.2 Making animation for dynamic field distribution

By using the files "@up", animation of the field distribution can be constructed. Type simply, "anime". Then 12 files named "@@?" are constructed where "?" is 0 to b indicating time sequence during the one cycle. Their data format is

$X_3 + u_3$, $X_1 + u_1$, u_2

Note u_i are normalized so that the maximum to be $0.3p$. Between lines with different X_3, line is inserted so as to display mesh in "gnuplot" software. Then by using the free software "GNUPLOT", the field distribution for u_i can be displayed by,

```
gnuplot> load "tools/anime/anime.plt"
```