Program for Calculating Discrete Green Function on Metallic Grating with Finite Thickness

FEMSDA Version 3.1

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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 fully periodic metallic grating structures with finite thickness by the use of discrete Green function theory. The finite element method (FEM) is employed for the electrode region, and distance among the FEM sampling points are weighted so as to make the convergence rapid. In the program, electrode cross section is assumed to be rectangular for simplicity. Supported substrate materials are $LiNbO_3$, $LiTaO_3$, $Li_2B_7O_4$, GaAs, quartz, $La_3Ga_5SiO_{12}$ and $KNbO_3$, with either Al, Au and Cu as the grating metal.

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 "femsda" 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 and the effective permittivity $\epsilon(\infty)/\epsilon_0$ of the substrate. If the piezoelectricity is decoupled, the program displays its situation and returns to step 2.

4. " Enter 1 for Al, 2 for Au or 3 for Cu" to specify the film material "& Enter 0 for OG (Open-Circuit Grating) or 1 for SG (Short-Circuited Grating" to specify the electrical condition. Then the program prints two bulk wave velocities in the film.

5. "Enter Nmax, Nxd, Nyd, fs, vnorm, w/p, and h/p" where w, p, h are the strip line-width, periodicity and height (see Fig. 1). The integer N_{max} represents the number of Floquet expansions to be included for the calculation. The integers N_{xd} and N_{yd} represent numbers of FEM subdivions for $w/2$ and h, respectively. The value V_{norm} represents arbitrary value used for the frequency normalization. Hereafter the operation frequency is normalized by V_{norm}/p. The value f_s is the relative frequency used only for finding initial value of the SAW velocity in the next step. For returning to step 2, enter "0 0 0 0 0 0 0".

6. "Enter vrs, vre and vrint" where V_{rs}, V_{re}, and V_{rint} are the start, end and interval, respectively, of velocities for searching initial values of the SAW velocity manually. Then "Enter als, ale and alint" where α_s, α_e, and α_{int} are the start, end and interval, respectively, of attenuation in dB for the search. After typing, the program tabulates velocities, attenuation and calculated determinants (complex value). The velocity giving zero determinant corresponds to the SAW velocity for specified f_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 fs, fe, fint, vstart and alpha" where f_s, f_e, f_{int} are the start, end and interval, respectively, of frequencies where the SAW properties are to be estimated. V_{start} and α are approximate values of the SAW velocity and attenuation in dB for $f = f_s$, and is estimated in the previous step. After typing, the program tabulates relative frequency, determined velocity (m/sec), attenuation (dB/λ), complex K^2, the reflection coefficient for

the semi-inifinite grating, propagation loss (dB/λ), and absolute value of the calculated determinant. These values are displayed and stored simultaneously into the file specified in the first step. Preceding the tabulated data, specified values and $\epsilon(\infty)/\epsilon_0$ are also listed. When all of the iteration complete, the program reexecutes this step. For returning to step 2, enter "0 0 0 0".

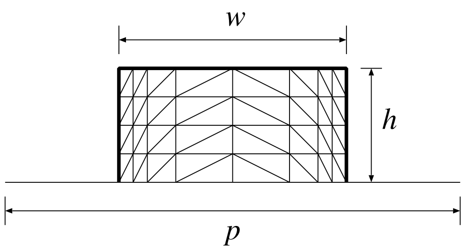

Figure 1: FEM mesh. In this case, $w/p = 0.5$, $h/p = 0.125$, $N_{xd} = 4$ and $N_{yd} = 4$.

2.1 Note

1. 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 the frequency is too close to the stopband edge.

2. Since piezoelectricity disappears at the frequency corresponding to the upper and lower edges of the stopband for the OC and SC gratings, respectively, it is actually impossible to determine SAW properties at the frequency. Since negative V_{int} is allowed, behaviour near the frequency can be determined by calculating SAW properties from frequencies higher than the stopband.

3. Although the reason is uncertain, even "Nmax" and "Nxd" should be used for fast convergence.

4. Maximum values of "Nxd", and "Nyd" are limited by available memory size of user's computer. That is, they must satisfy following relations:

$$2(2 \times \mathrm{Nxd} + 1) \times (\mathrm{Nyd} + 1) \leq \mathrm{npm}$$

   and

$$2 \times \mathrm{Nxd} + 1 \leq \mathrm{npa}$$

   where "npm" and "npa" are the parameters defined in the software sourcecode. Note that their default values are 300 and 100, respectively.

5. From version 2.0, very simple but quite effective trick was introduced to be able to find solutions easily even when the piezoelectricity is weak and/or attenuation is quite large. As a trade-off, criterion in the step 7 to stop further iteration becomes weak. So validity of the result should be checked by the determinant. It should be converged at least 10^{-5}.

6. 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 "femsda.f".

7. In the software, the electrode cross section is assumed to be rectangular. The software is also able to analyze the trapezoid case by specifying the parameter "aspect" in the main routines in "femsda.f". Note that "aspect" is defined by $(b-a)/h$ where a and b are the upper and lower lengths, respectively, and h is the electrode height.

3 Field distribution

Data format

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

X_3, X_1, u_1, u_2, u_3 and $10^{-10}\phi$

where u_i and ϕ are complex values. Between lines with different X_3, a blank line is inserted so as to display mesh in "gnuplot" software. In "@ue", the distribution in the film is tabulated. The data format is,

X_3, X_1, u_1, u_2, and u_3.

In both files, numbers of points calculated toward X_1 and X_3 are given at first line.

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, $\Re(u_2)$ can be displayed by,

```
gnuplot> set data style lines
gnuplot> set ticslevel 0
gnuplot> splot "@up" using 1:2:5, "@ue" using 1:2:5
```

If you do not have the software, you can get through most of all anonymous ftp server. Note the software works both UNIX and Windows environments. subsectionMaking animation for dynamic field distribution By using the files "@up" and "@ue", animation of the field distribution can be made. Type simply, "animeg". Then 12 files named "@@?" and other "@@e?" are constructed where "?" is 0 to b indicating time sequence during the one cycle. The former files are for the substrate and the latter files are for the film. 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 $0.1p$. 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/anime3D.plt"
```

If you want to see field distribution in $X_1 - X_3$ plane and u_2 is out of interest, you can display the motion two dimensionally by using the same output using the same output. This is done again by using the "GNUPLOT" through,

```
gnuplot> load "tools/anime/anime2D.plt"
```

If you want to display ϕ instead of u_i, run "animep". Then 12 files named "@@?" are constructed. The data format is the same with above. Then the field distribution for u_i can be displayed by,

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