# Quartz Transducer Modeling for Development of BAW Resonators

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## 1. Introduction

Transducer optimization is a key aspect for successful development and deployment of advanced sensors, especially when designing 3D structures for harsh environments. Quartz has been the material of choice for the fabrication of bulk acoustic wave (BAW) devices, which are used for measurement of many quantities, such as, temperature, pressure, acceleration, mass.

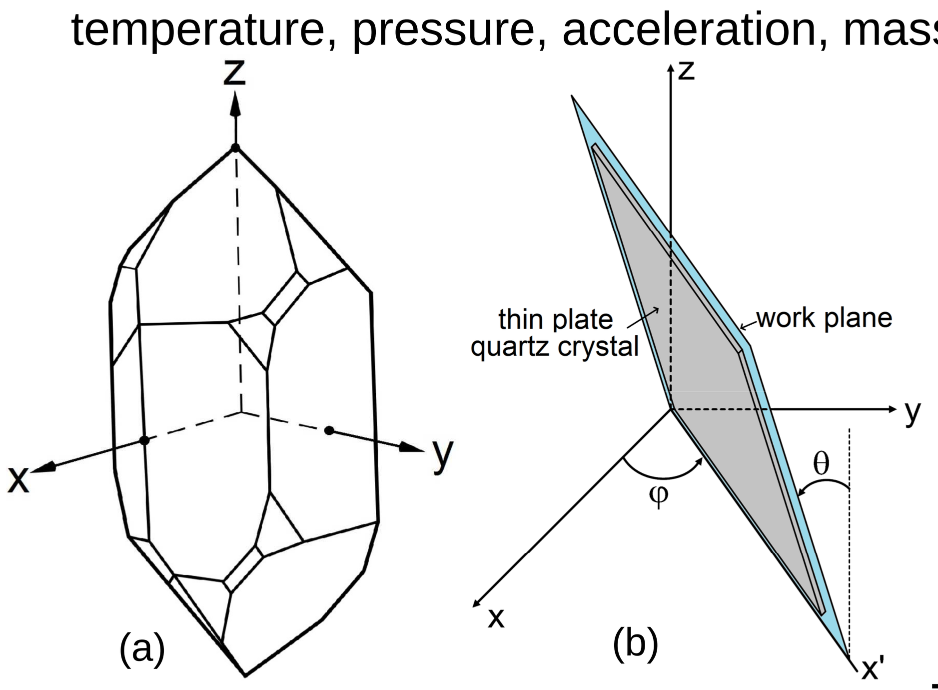


**Figure 1**. (a) Coordinate system adopted in the crystal. (b) Double rotated cut angles.

| θ(°) | φ(°) | cut |
|---|---|---|
| -60 | 0 | BC |
| -57 | 0 | FT |
| -49 | 0 | BT |
| 31 | 0 | AC |
| 35.25 | 0 | AT |
| 38 | 0 | CT |
| 42.75 | 0 | ST |
| 66.5 | 0 | ET |
| 35.25 | 21.9 | SC |

**Table 1**. Quartz cut for the shear thickness vibration modes.

## Flowchart

**Startup settings:**
**Space dimension:** 2D or 3D
**Physics:** Piezoelectric Devices
**Studies:** Eigenfrequency and frequency domain

↓

**Draw the structure**

↓

**Set the constants ρ, [c], [e] and [ε]**

↓

**Set the boundary conditions**

↓

**Set the mesh**

↓

**Set the parameters for each study**

↓

**Show the deformations and plot admittance curve**

## 2. Theory

The piezoelectric coupling can be represented mathematically through the constitutive relations of piezoelectricity:

$$D_i = e_{ijk} S_{jk} + \varepsilon_{ij} E_j \qquad T_{ij} = c_{ijkl} S_{kl} - e_{kij} E_k$$

The eigenfrequency equation for the harmonics is given by following equation:

$$f_n = n\frac{v}{2h}, \quad n = 1,3,5,\ldots \qquad v = \sqrt{\frac{\bar{c}_{66}}{\rho}}, \quad \bar{c}_{66} = c_{66}\left(1 + k_{26}^2\right) \qquad k_{26}^2 = \frac{e_{26}^2}{c_{66}\varepsilon_{22}}$$

$$f_1(\theta) = \frac{1}{2h}\sqrt{\frac{c_{66}\cos^2(\theta) + c_{44}\sin^2(\theta) + 2c_{14}\sin(\theta)\cos(\theta)}{\rho}}$$

| Material | $k_{26}^2$ (%) |
|---|---|
| Quartz | 0,78 |
| AlN | 6,5 |
| ZnO | 7,5 |

## 3. 2D Analysis and results

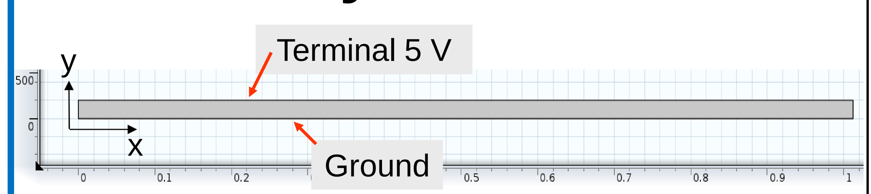


**Figure 2**. 2D Geometry: 10115.28 × 200 µm.

$$[c] = \begin{bmatrix} 86.74 & -8.25 & 27.15 & -3.66 & 0 & 0 \\ -8.25 & 129.77 & -7.42 & 5.7 & 0 & 0 \\ 27.15 & -7.42 & 102.83 & 9.92 & 0 & 0 \\ -3.66 & 5.7 & 9.92 & 38.61 & 0 & 0 \\ 0 & 0 & 0 & 0 & 68.81 & 2.53 \\ 0 & 0 & 0 & 0 & 2.53 & 29.01 \end{bmatrix} \times 10^9 \ \mathrm{N/m^2}$$

$$[e] = \begin{bmatrix} 17.1 & -15.2 & -1.87 & 6.7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 10.8 & -9.5 \\ 0 & 0 & 0 & 0 & -7.61 & 6.7 \end{bmatrix} \times 10^{-2} \ \mathrm{C/m^2}$$

$$[\varepsilon] = \begin{bmatrix} 39.21 & 0 & 0 \\ 0 & 39.82 & 0.86 \\ 0 & 0.86 & 40.42 \end{bmatrix} \times 10^{-12} \ \mathrm{C/Vm}$$

**Table 2**. Constants for AT-cut quartz.

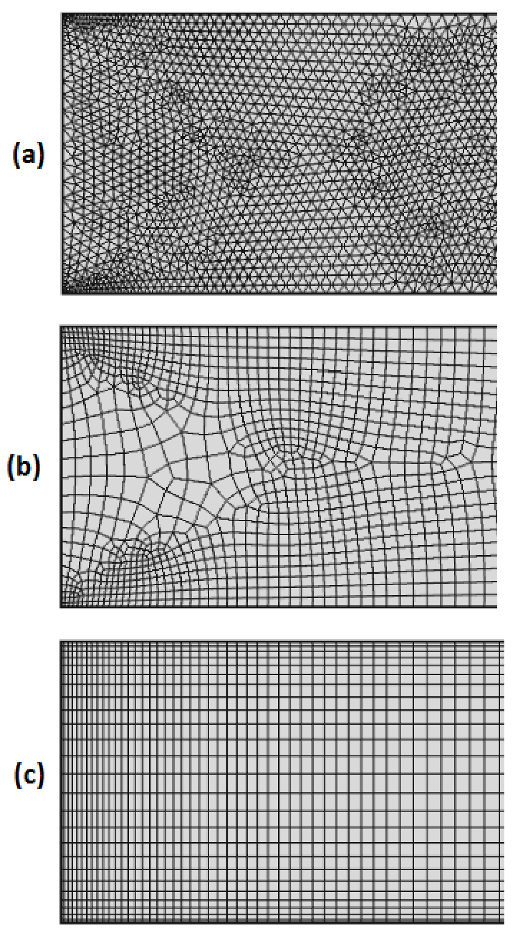


**Figure 3**. Meshes: free triangular (a), free quadratic (b) and mapped (c).

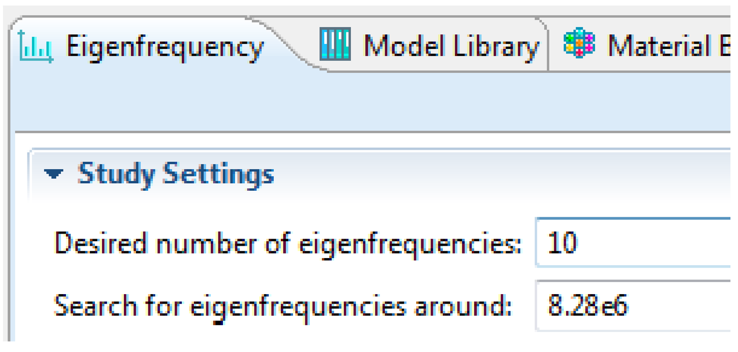


**Figure 4**. Eigenfrequency study settings.

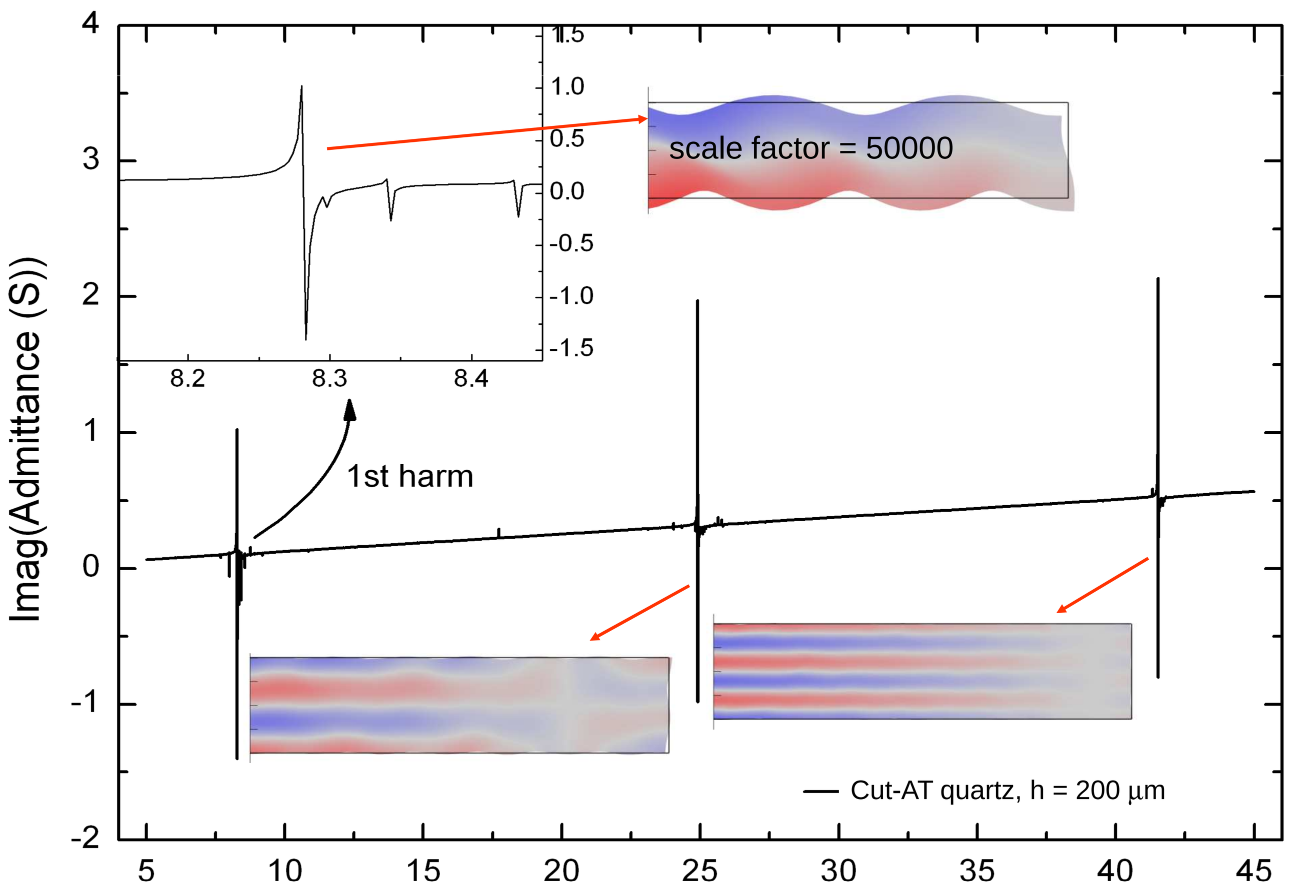


**Figure 5**. Frequency response and the displacements field (x-component) for AT-cut.

| | frequency (MHz) | | relative error (%) |
|---|---|---|---|
| | theory | COMSOL | |
| $f_1$ | 8.3054 | 8.2852 | 0.244 |
| $f_3$ | 24.9163 | 24.9103 | 0.024 |
| $f_5$ | 41.5272 | 41.5365 | 0.022 |

**Table 3**. Results with the AT-cut quartz constants.

## 4. 3D Analysis and results

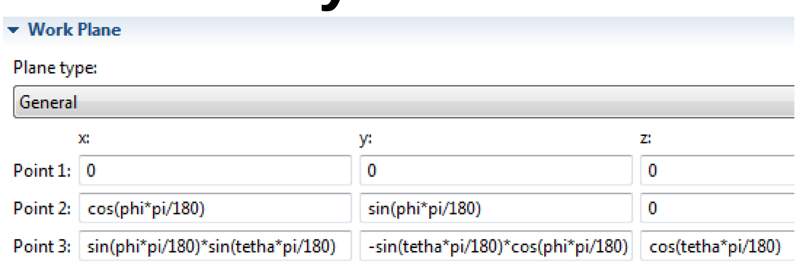


**Figure 6**. θ and φ in the work plane.

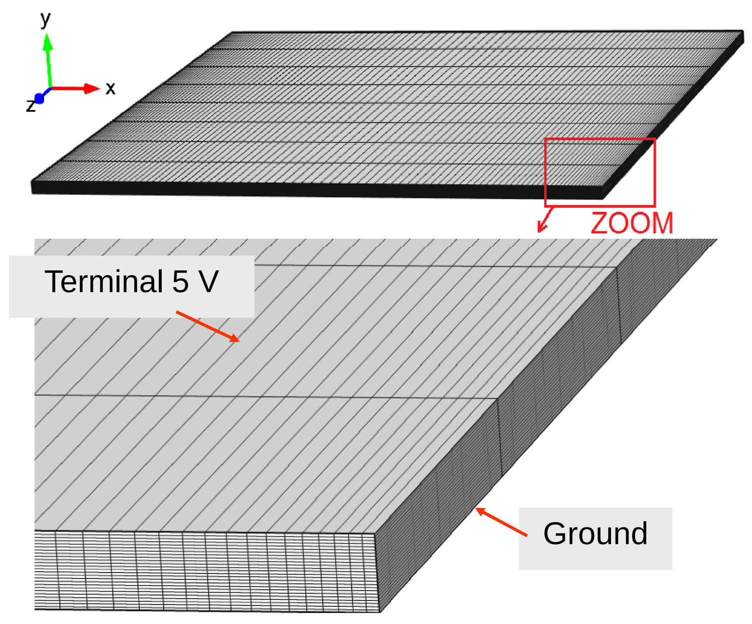


**Figure 7**. Mesh with 20000 (100 x 25 x 8) finite elements. 10115.28 × 10115.28 × 200 µm.

$$[c] = \begin{bmatrix} 86.74 & 6.99 & 11.91 & -17.91 & 0 & 0 \\ 6.99 & 86.74 & 11.91 & 17.91 & 0 & 0 \\ 11.91 & 11.91 & 107 & 0 & 0 & 0 \\ -17.91 & 17.91 & 0 & 57.94 & 0 & 0 \\ 0 & 0 & 0 & 0 & 57.94 & -17.91 \\ 0 & 0 & 0 & 0 & -17.91 & 39.88 \end{bmatrix} \times 10^9 \ \mathrm{N/m^2}$$

$$[e] = \begin{bmatrix} 17.1 & -17.1 & 0 & -4.06 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4.06 & -17.1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \times 10^{-2} \ \mathrm{C/m^2}$$

$$[\varepsilon] = \begin{bmatrix} 39.21 & 0 & 0 \\ 0 & 39.21 & 0 \\ 0 & 0 & 41.03 \end{bmatrix} \times 10^{-12} \ \mathrm{C/Vm}$$

**Table 4**. Constants for left-handed quartz .

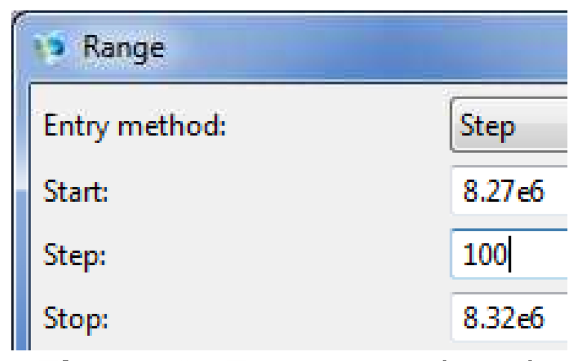


**Figure 8**. Frequency domain study settings.

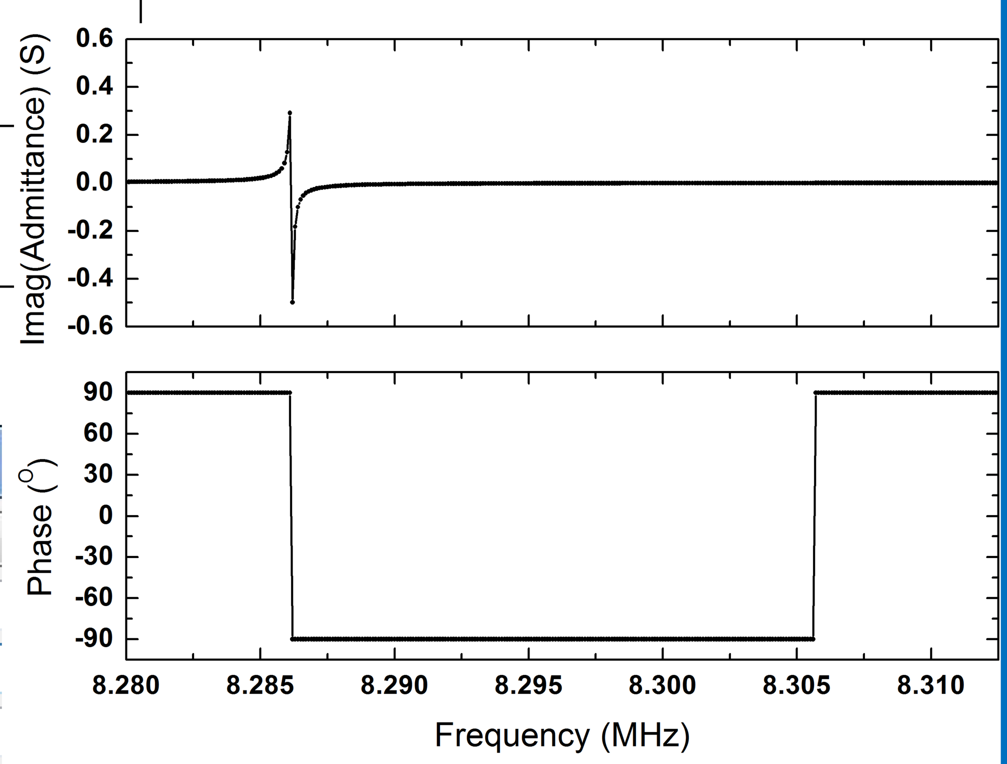


**Figure 9**. Frequency response for the first harmonic. θ = 35.25° and φ = 0°. A step of 100 Hz is performed.

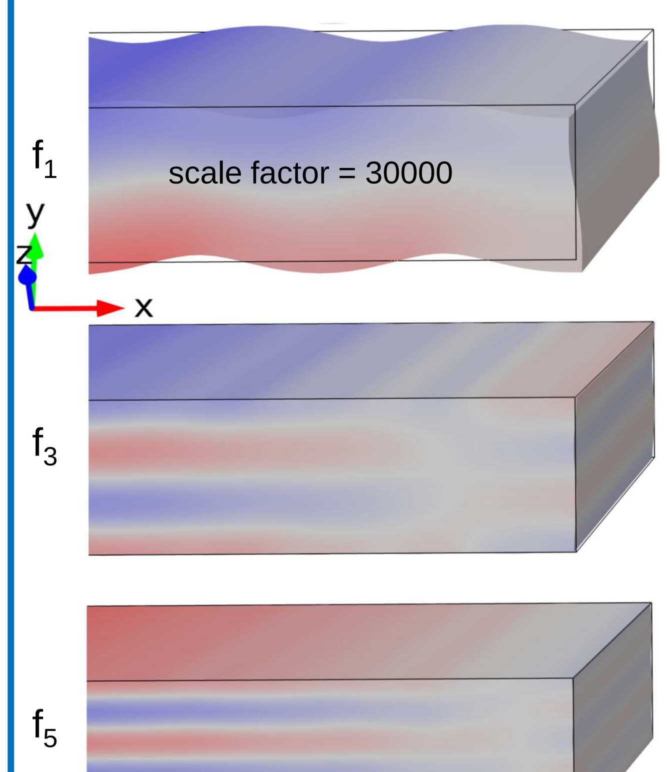


**Figure 10**. Displacement field (x-component). θ = 35.25° and φ = 0°.

| θ(°) | cut | frequency (MHz) | | | |
|---|---|---|---|---|---|
| | | theory | COMSOL | | |
| | | $f_1(\theta)$ | $f_1$ | $f_3$ | $f_5$ |
| -60 | BC | 12.7532 | 12.7595 | 38.2878 | 63.8457 |
| -57 | FT | 12.7541 | 12.7605 | 38.2962 | 63.8461 |
| -49 | BT | 12.6573 | 12.6664 | 38.0314 | 63.3996 |
| 31 | AC | 8.2513 | 8.2650 | 24.8696 | 41.4638 |
| 35.25 | AT | 8.2736 | 8.2855 | 24.9105 | 41.5292 |
| 38 | CT | 8.3211 | 8.3318 | 25.0377 | 41.7396 |
| 42.75 | ST | 8.4616 | 8.4723 | 25.4359 | 42.4009 |
| 66.5 | ET | 9.9510 | 9.9539 | 29.8555 | 49.7641 |

**Table 5**. Results with the left handed quartz constants.

Electrical behavior near the resonance frequency:

$$f_s = \frac{1}{2\pi\sqrt{LC}} \qquad f_p = f_s\left(1 + \frac{C}{2C_0}\right) \qquad C_0 = \frac{\varepsilon_{22} a^2}{h} \qquad Q = \frac{\omega_s}{\Delta\omega_{3dB}} = \frac{1}{R}\sqrt{\frac{L}{C}}$$

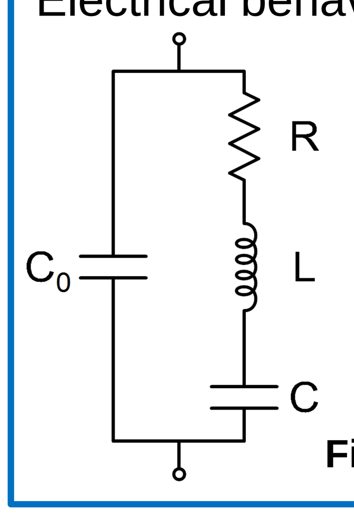


**Figure 11**. Equivalent circuit.

| step (Hz) | R (Ω) | L (mH) | C (fF) | Q |
|---|---|---|---|---|
| 20 | 0.111801 | 3.913113 | 94.277723 | 1822270.76 |
| 100 | 2.003140 | 3.921181 | 94.083282 | 101915.66 |
| 500 | 7.810364 | 3.901143 | 94.571102 | 26004.32 |

**Table 6**. Extraction of parameters. $C_0$ = 20.069107 pF.

## 5. Conclusions

A thin quartz plate has been simulated in 2D and 3D and the results are in good agreement. It was shown that the displacements occurred in the x-direction, and that the shear thickness vibration mode are presented. Next, the damping will be included in the simulation to get correct equivalent circuit parameters and quality factor. There is also interest in evaluating the effect of the electrodes on the transducer, and analyze other 3D geometries. With COMSOL, it expected to save design time before performing the actual maching of the quartz blank.

## 6. References

1. J. Yang, Analysis of piezoelectric devices. World Scientific (2006).
2. K. Lakin, A Review of Thin-Film Resonator Technology, *IEEE Microwave Magazine*, **4**, no. 4, 61 (2003).