Introduction to SAWAVE

A 3D Based Surface Acoustic Wave (SAWAVE) Device Simulator

NovaTCAD

20 years ANNIVERSARY

CROSSLIGHT

SAWAVE FV Data Structure

- Unstructured Finite Volume (FV) mesh allows unparalleled flexibility in 3D structure definition.
- Efficient 3D stress solver with GPU acceleration (optional).
- Convenient 3D GUI allows use of GDSII mask layout format.
- Compatible with all existing Crosslight device simulators.
- Efficient wave solver uses coupled mode theory, incorporating results from 3D stress solver.
- Convenient graphic output using CrosslightView (OpenGL-based).

SAWAVE Input Data

- 3D metal and piezoelectrical crystal geometry and mesh definition for single or multiple periods.

- SAW device segments along wave propagation direction (number of periods of interdigital finger, or IDF), with or without acoustic grating. Open or short circuit IDF.

- Stiffness matrix parameters (Young’s modulus, Poisson’s ratio and shear modulus), piezoelectric parameter tensors and mass densities conveniently collected in material libraries for commonly-used SAW materials.

- Crystal cut rigorously described by miller indices.

- Wave reflectivity at both ends of SAW device.

- Frequency range and number of frequency data points required.

SAWAVE Output Data

- All 3D displacement vectors and stress components excited by input AC bias (such as Sxx, Sxy, Syy, Szz, etc.), obtained rigorously from the FV stress solver.

- SAW lateral mode averaged Rayleigh wave vector as a function of position along the propagation direction; used to extract coupling coefficient kappa

- SAW lateral mode averaged piezo stress source distribution used to perform Green’s function analysis for the whole multiple period device.

- Rayleigh wave amplitude distribution in the whole device.

- Y and S parameters, reflection and transmission coefficients versus frequency.

SAWAVE Easy to Use GUI

- Mature and integrated UI.
- Automatic input lookup and assistance.
- Large number of examples.
- Large material database.
- Automated series of simulation and design of experiment (DOE).

Basic equations

$$-\omega^2 \rho u_i = \frac{\partial}{\partial x_j}\left[\left(c_{ijkl}\frac{\partial u_k}{\partial x_l}\right) + e_{ijk}\frac{\partial \Phi}{\partial x_k}\right]$$

$$D_i = e_{ijk}\frac{\partial u_j}{\partial x_k} - \varepsilon_{ij}\frac{\partial \Phi}{\partial x_j}$$

Plus the usual Poisson's equation and the current continuity equations, for both DC and AC analysis (ref: Chen and Haus, IEEE Trans Sonic and Ultrasonic, vol. SU-32, p395, 1985)

Elastic stiffness tensor c_{ijkl}

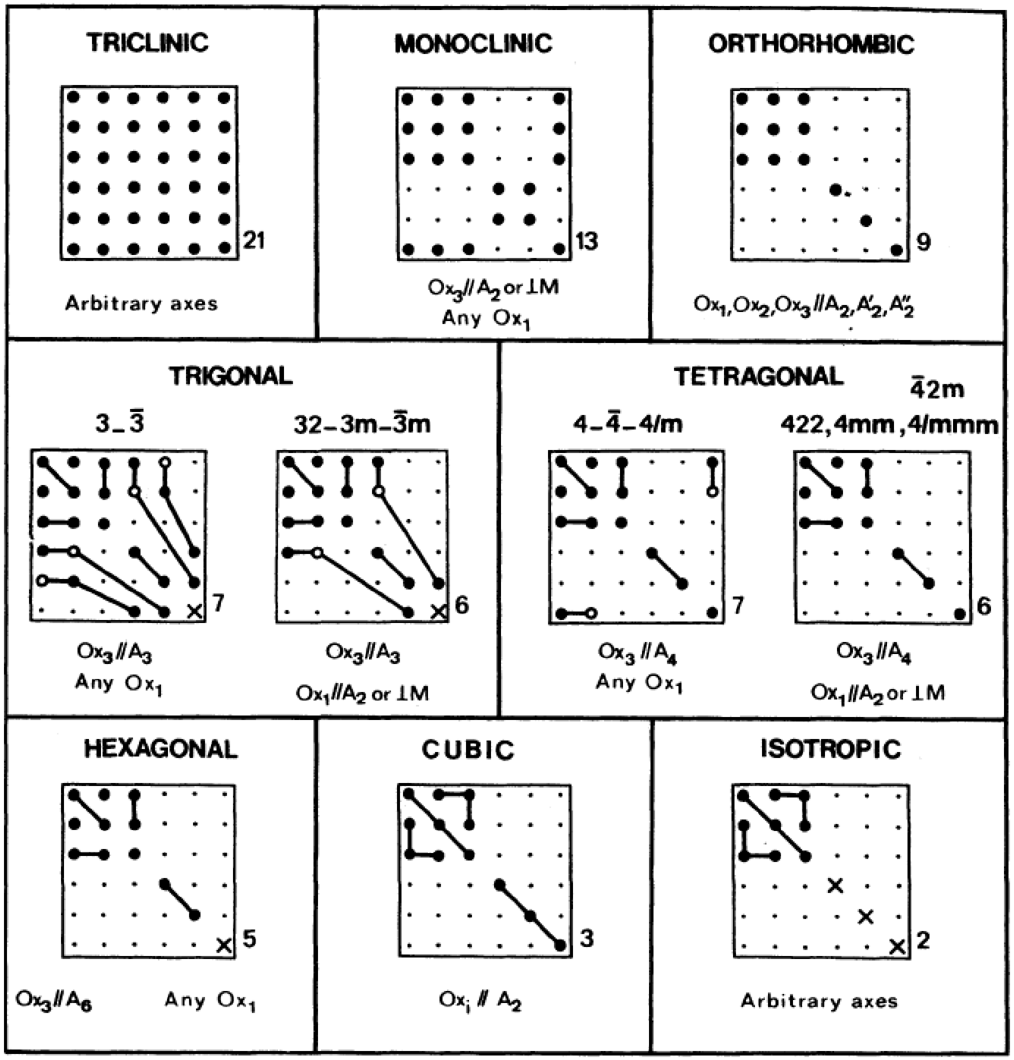
$$c_{\alpha\beta} = \begin{vmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{21} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{31} & c_{32} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{41} & c_{42} & c_{43} & c_{44} & c_{45} & c_{46} \\ c_{51} & c_{52} & c_{53} & c_{54} & c_{55} & c_{56} \\ c_{61} & c_{62} & c_{63} & c_{64} & c_{65} & c_{66} \end{vmatrix}$$

36 independent elastic constants due to symmetry

A pair of unordered indices (i, j) can give 6 independent values

$$\begin{array}{ccc} (11) \leftrightarrow 1 & (22) \leftrightarrow 2 & (33) \leftrightarrow 3 \\ (23) = (32) \leftrightarrow 4 & (31) = (13) \leftrightarrow 5 & (12) = (21) \leftrightarrow 6 \end{array} .$$

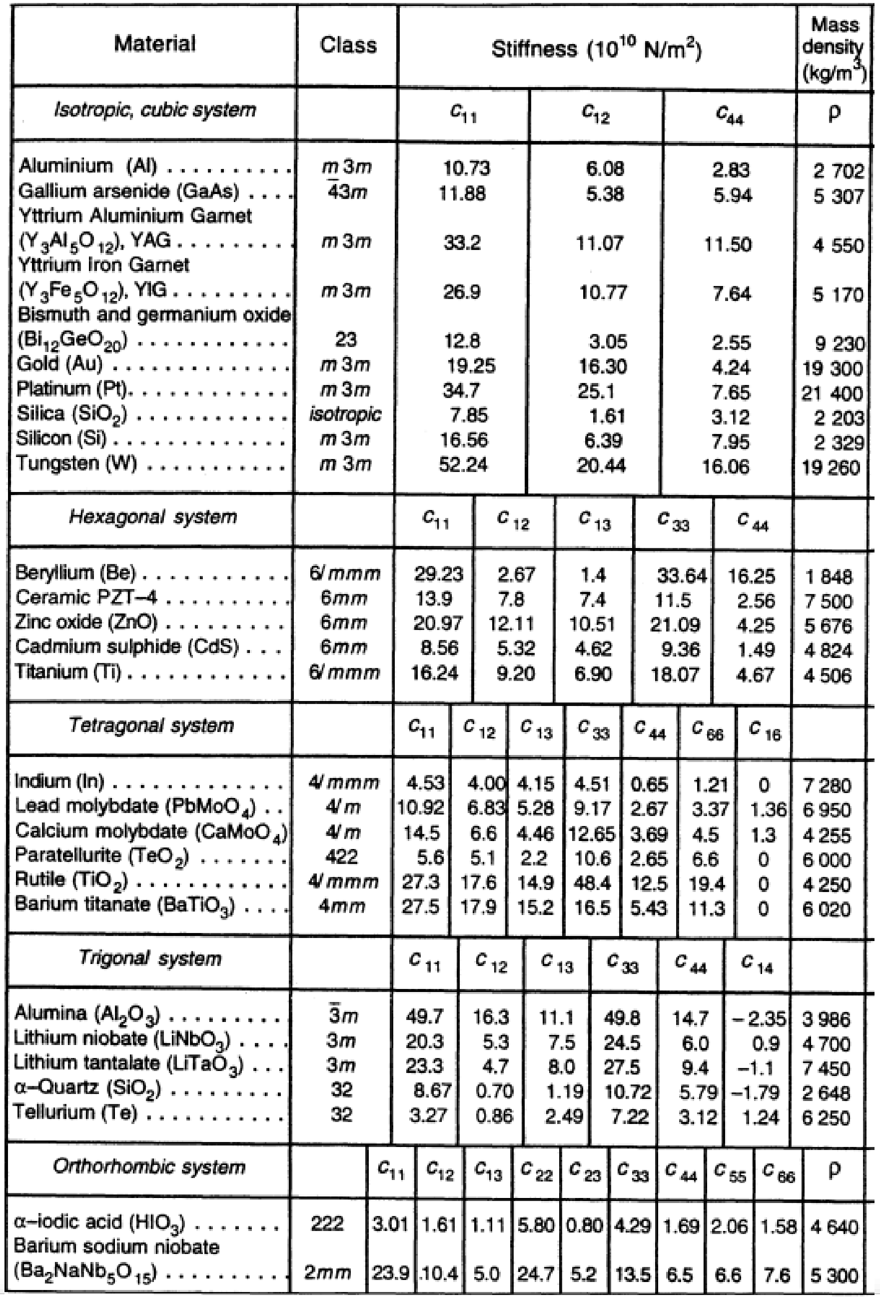
Effect of Crystal Symmetry on c_{ijkl}



Relations between components $c_{\alpha\beta}$ of the elastic stiffness tensor for different crystal classes.

· : zero component,
●—○ : equal and opposite components,
● ○ : non-zero component,
●—● : equal components,
× : component equal to $(c_{11} - c_{12})/2$.

Ref. Daniel Royer, Eugène Dieulesaint, “Elastic Waves in solids I Free and Guided Propagation”, Springer



Material	Class	Stiffness (10^{10} N/m^2)									Mass density (kg/m^3)
Isotropic, cubic system		c_{11}	c_{12}	c_{44}							ρ
Aluminium (Al)	m3m	10.73	6.08	2.83							2 702
Gallium arsenide (GaAs)	$\bar{4}3m$	11.88	5.38	5.94							5 307
Yttrium Aluminium Garnet ($Y_3Al_5O_{12}$), YAG	m3m	33.2	11.07	11.50							4 550
Yttrium Iron Garnet ($Y_3Fe_5O_{12}$), YIG	m3m	26.9	10.77	7.64							5 170
Bismuth and germanium oxide ($Bi_{12}GeO_{20}$)	23	12.8	3.05	2.55							9 230
Gold (Au)	m3m	19.25	16.30	4.24							19 300
Platinum (Pt)	m3m	34.7	25.1	7.65							21 400
Silica (SiO_2)	isotropic	7.85	1.61	3.12							2 203
Silicon (Si)	m3m	16.56	6.39	7.95							2 329
Tungsten (W)	m3m	52.24	20.44	16.06							19 260
Hexagonal system		c_{11}	c_{12}	c_{13}	c_{33}	c_{44}					
Beryllium (Be)	6/mmm	29.23	2.67	1.4	33.64	16.25					1 848
Ceramic PZT–4	6mm	13.9	7.8	7.4	11.5	2.56					7 500
Zinc oxide (ZnO)	6mm	20.97	12.11	10.51	21.09	4.25					5 676
Cadmium sulphide (CdS)	6mm	8.56	5.32	4.62	9.36	1.49					4 824
Titanium (Ti)	6/mmm	16.24	9.20	6.90	18.07	4.67					4 506
Tetragonal system		c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{66}	c_{16}			
Indium (In)	4/mmm	4.53	4.00	4.15	4.51	0.65	1.21	0			7 280
Lead molybdate ($PbMoO_4$)	4/m	10.92	6.83	5.28	9.17	2.67	3.37	1.36			6 950
Calcium molybdate ($CaMoO_4$)	4/m	14.5	6.6	4.46	12.65	3.69	4.5	1.3			4 255
Paratellurite (TeO_2)	422	5.6	5.1	2.2	10.6	2.65	6.6	0			6 000
Rutile (TiO_2)	4/mmm	27.3	17.6	14.9	48.4	12.5	19.4	0			4 250
Barium titanate ($BaTiO_3$)	4mm	27.5	17.9	15.2	16.5	5.43	11.3	0			6 020
Trigonal system		c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{14}				
Alumina (Al_2O_3)	$\bar{3}m$	49.7	16.3	11.1	49.8	14.7	−2.35				3 986
Lithium niobate ($LiNbO_3$)	3m	20.3	5.3	7.5	24.5	6.0	0.9				4 700
Lithium tantalate ($LiTaO_3$)	3m	23.3	4.7	8.0	27.5	9.4	−1.1				7 450
α–Quartz (SiO_2)	32	8.67	0.70	1.19	10.72	5.79	−1.79				2 648
Tellurium (Te)	32	3.27	0.86	2.49	7.22	3.12	1.24				6 250
Orthorhombic system		c_{11}	c_{12}	c_{13}	c_{22}	c_{23}	c_{33}	c_{44}	c_{55}	c_{66}	ρ
α–iodic acid (HIO_3)	222	3.01	1.61	1.11	5.80	0.80	4.29	1.69	2.06	1.58	4 640
Barium sodium niobate ($Ba_2NaNb_5O_{15}$)	2mm	23.9	.10.4	5.0	24.7	5.2	13.5	6.5	6.6	7.6	5 300

Elastic stiffness constants and mass densities for various crystals, organized according to crystal class.

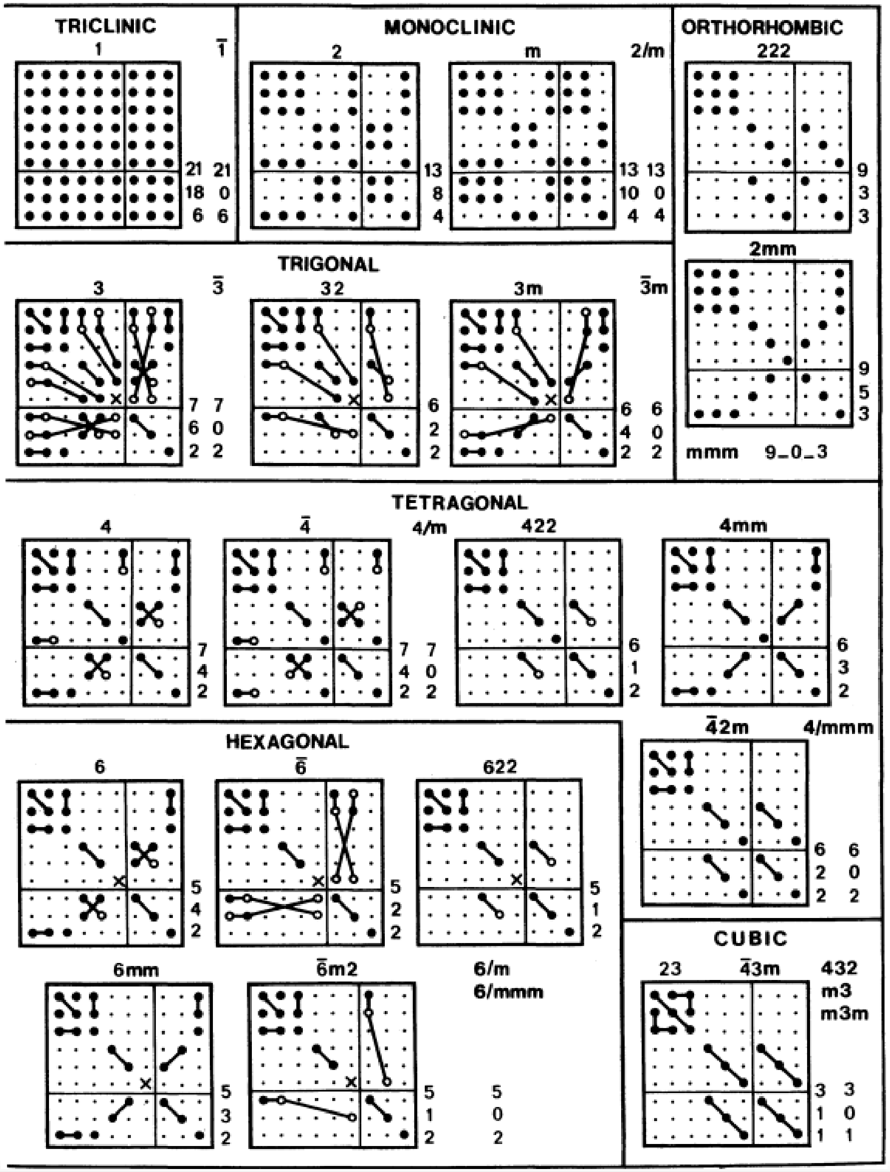
Ref. Daniel Royer, Eugène Dieulesaint, “Elastic Waves in solids I Free and Guided Propagation”, Springer

Piezoelectric tensor e_{ijk}

$$e_{i\alpha} = \begin{vmatrix} e_{11} & e_{12} & e_{13} & e_{14} & e_{15} & e_{16} \\ e_{21} & e_{22} & e_{23} & e_{24} & e_{25} & e_{26} \\ e_{31} & e_{32} & e_{33} & e_{34} & e_{35} & e_{36} \end{vmatrix}$$

Independent piezoelectric constants reduced from 27 to 18 due to symmetry

Effect of Crystal Symmetry on e_{ijk}

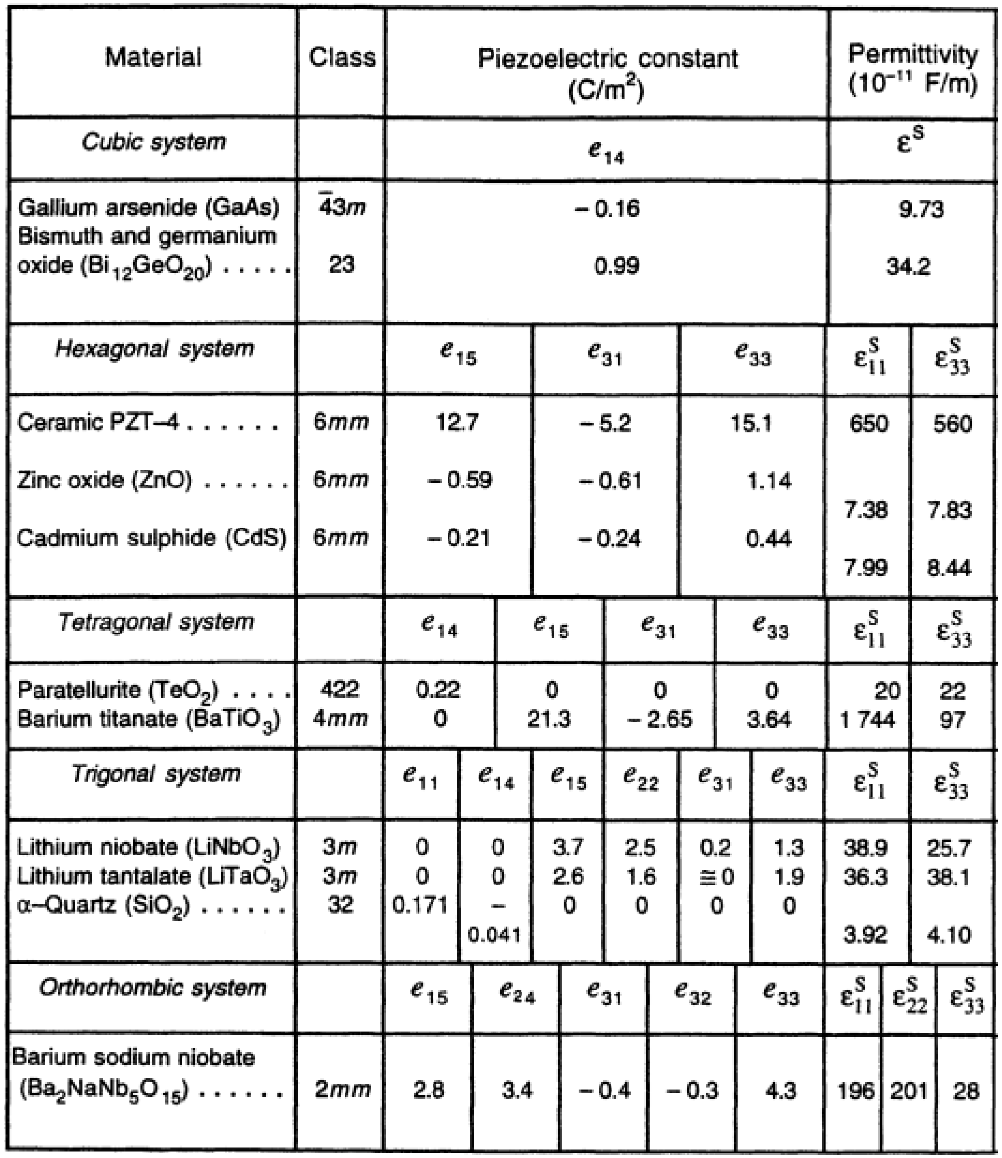


Components of the elastic, piezoelectric and dielectric tensors, organized according to symmetry class,

. : zero component,
●—○ : equal and opposite components,
● ○ : non-zero component,
●—● : equal components,
× : component equal to $(c_{11} - c_{12})/2$.

Ref. Daniel Royer, Eugène Dieulesaint, “Elastic Waves in solids I Free and Guided Propagation”, Springer

NovaTCAD



Material	Class	Piezoelectric constant (C/m^2)	Permittivity $(10^{-11}$ F/m)
Cubic system		e_{14}	ε^S
Gallium arsenide (GaAs)	$\bar{4}3m$	−0.16	9.73
Bismuth and germanium oxide ($Bi_{12}GeO_{20}$)	23	0.99	34.2

Hexagonal system		e_{15}	e_{31}	e_{33}	ε^S_{11}	ε^S_{33}
Ceramic PZT–4	6*mm*	12.7	−5.2	15.1	650	560
Zinc oxide (ZnO)	6*mm*	−0.59	−0.61	1.14	7.38	7.83
Cadmium sulphide (CdS)	6*mm*	−0.21	−0.24	0.44	7.99	8.44

Tetragonal system		e_{14}	e_{15}	e_{31}	e_{33}	ε^S_{11}	ε^S_{33}
Paratellurite (TeO_2)	422	0.22	0	0	0	20	22
Barium titanate ($BaTiO_3$)	4*mm*	0	21.3	−2.65	3.64	1 744	97

Trigonal system		e_{11}	e_{14}	e_{15}	e_{22}	e_{31}	e_{33}	ε^S_{11}	ε^S_{33}
Lithium niobate ($LiNbO_3$)	3*m*	0	0	3.7	2.5	0.2	1.3	38.9	25.7
Lithium tantalate ($LiTaO_3$)	3*m*	0	0	2.6	1.6	≅0	1.9	36.3	38.1
α–Quartz (SiO_2)	32	0.171	−0.041	0	0	0	0	3.92	4.10

Orthorhombic system		e_{15}	e_{24}	e_{31}	e_{32}	e_{33}	ε^S_{11}	ε^S_{22}	ε^S_{33}
Barium sodium niobate ($Ba_2NaNb_5O_{15}$)	2*mm*	2.8	3.4	−0.4	−0.3	4.3	196	201	28

Piezoelectric and dielectric constants for crystals, classified by crystal system

Ref. Daniel Royer, Eugène Dieulesaint, “Elastic Waves in solids I Free and Guided Propagation”, Springer

Stress equations

$$\sigma_{ij} = c_{ijkl}\frac{\partial u_l}{\partial x_k}$$

$$\sigma_{xx} = C_{11}\frac{\partial u}{\partial x} + C_{12}\frac{\partial v}{\partial y} + C_{13}\frac{\partial w}{\partial z} + C_{14}\frac{\partial w}{\partial y} + C_{14}\frac{\partial v}{\partial z} + C_{15}\frac{\partial w}{\partial x} + C_{15}\frac{\partial u}{\partial z} + C_{16}\frac{\partial v}{\partial x} + C_{16}\frac{\partial u}{\partial y}$$

$$\sigma_{yy} = C_{21}\frac{\partial u}{\partial x} + C_{22}\frac{\partial v}{\partial y} + C_{23}\frac{\partial w}{\partial z} + C_{24}\frac{\partial w}{\partial y} + C_{24}\frac{\partial v}{\partial z} + C_{25}\frac{\partial w}{\partial x} + C_{25}\frac{\partial u}{\partial z} + C_{26}\frac{\partial v}{\partial x} + C_{26}\frac{\partial u}{\partial y}$$

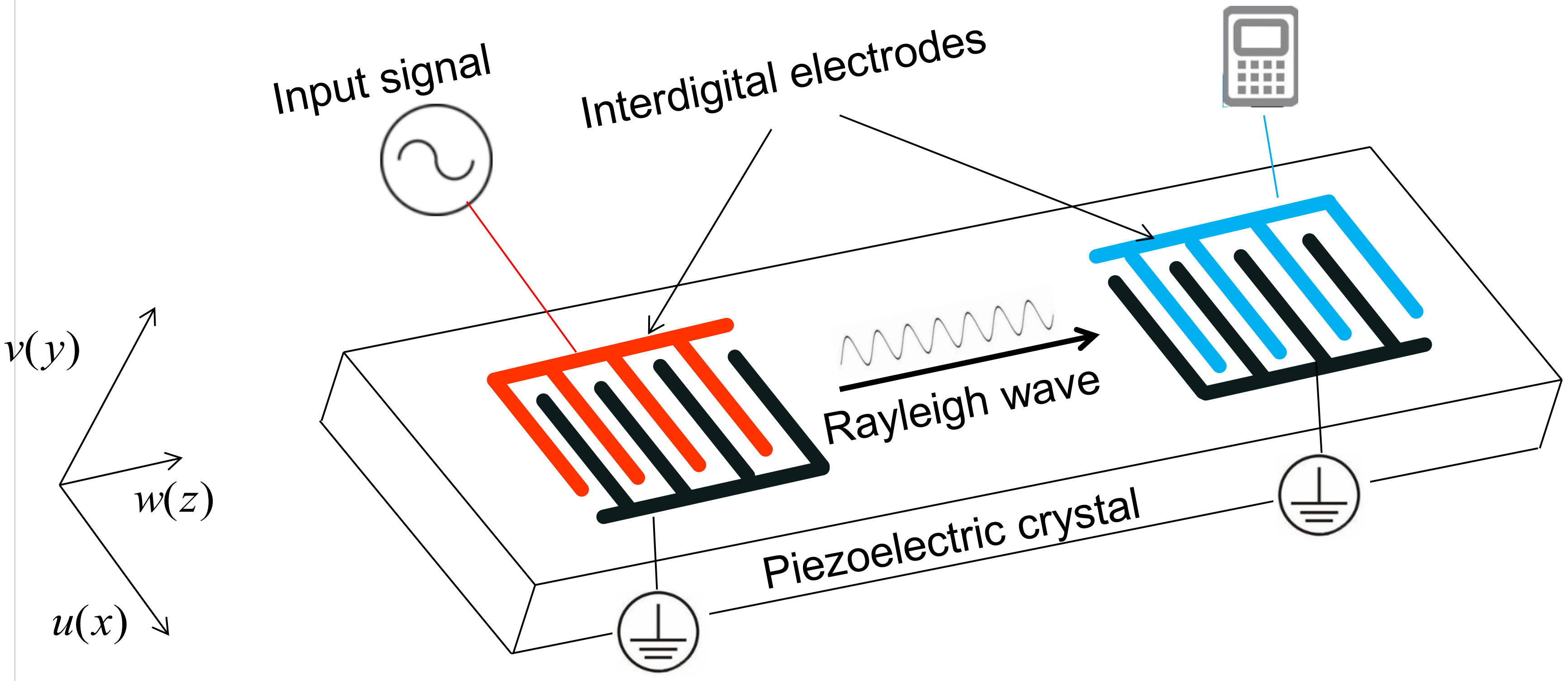
$$\sigma_{zz} = C_{31}\frac{\partial u}{\partial x} + C_{32}\frac{\partial v}{\partial y} + C_{33}\frac{\partial w}{\partial z} + C_{34}\frac{\partial w}{\partial y} + C_{34}\frac{\partial v}{\partial z} + C_{35}\frac{\partial w}{\partial x} + C_{35}\frac{\partial u}{\partial z} + C_{36}\frac{\partial v}{\partial x} + C_{36}\frac{\partial u}{\partial y}$$

$$\sigma_{xy} = \sigma_{yx} = C_{61}\frac{\partial u}{\partial x} + C_{62}\frac{\partial v}{\partial y} + C_{63}\frac{\partial w}{\partial z} + C_{64}\frac{\partial w}{\partial y} + C_{64}\frac{\partial v}{\partial z} + C_{65}\frac{\partial w}{\partial x} + C_{65}\frac{\partial u}{\partial z} + C_{66}\frac{\partial v}{\partial x} + C_{66}\frac{\partial u}{\partial y}$$

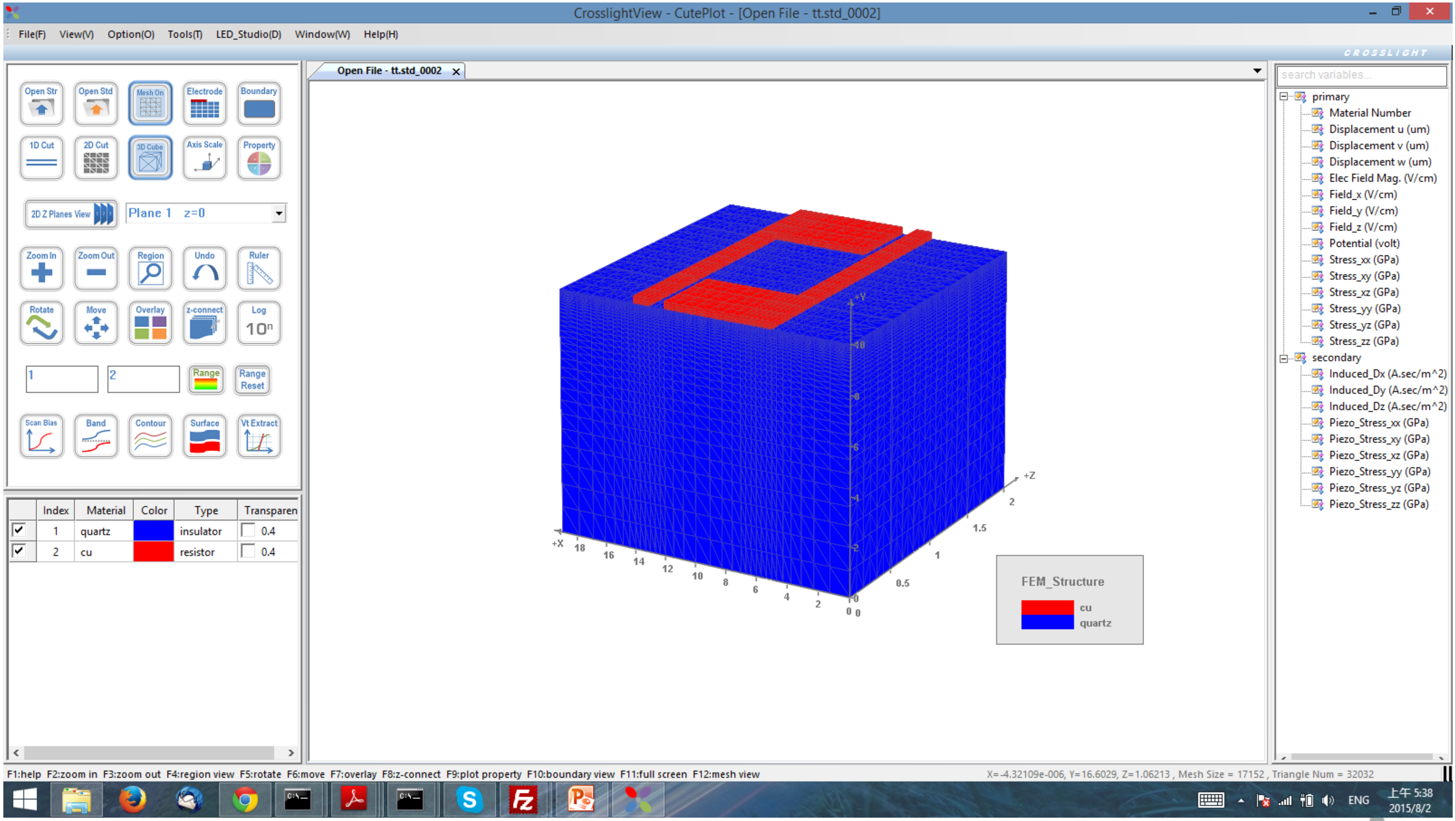
$$\sigma_{yz} = \sigma_{zy} = C_{41}\frac{\partial u}{\partial x} + C_{42}\frac{\partial v}{\partial y} + C_{43}\frac{\partial w}{\partial z} + C_{44}\frac{\partial w}{\partial y} + C_{44}\frac{\partial v}{\partial z} + C_{45}\frac{\partial w}{\partial x} + C_{45}\frac{\partial u}{\partial z} + C_{46}\frac{\partial v}{\partial x} + C_{46}\frac{\partial u}{\partial y}$$

$$\sigma_{zx} = \sigma_{xz} = C_{51}\frac{\partial u}{\partial x} + C_{52}\frac{\partial v}{\partial y} + C_{53}\frac{\partial w}{\partial z} + C_{54}\frac{\partial w}{\partial y} + C_{54}\frac{\partial v}{\partial z} + C_{55}\frac{\partial w}{\partial x} + C_{55}\frac{\partial u}{\partial z} + C_{56}\frac{\partial v}{\partial x} + C_{56}\frac{\partial u}{\partial y}$$

Typical SAW Structure



Simulated Structure

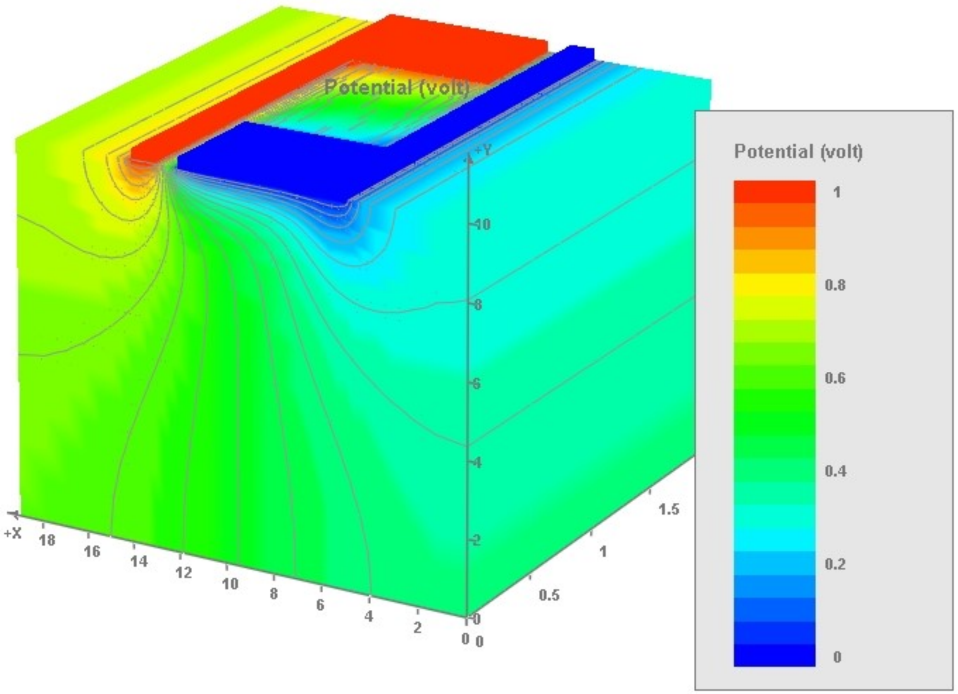


	Index	Material	Color	Type	Transparen
☑	1	quartz	🟦	insulator	☐ 0.4
☑	2	cu	🟥	resistor	☐ 0.4

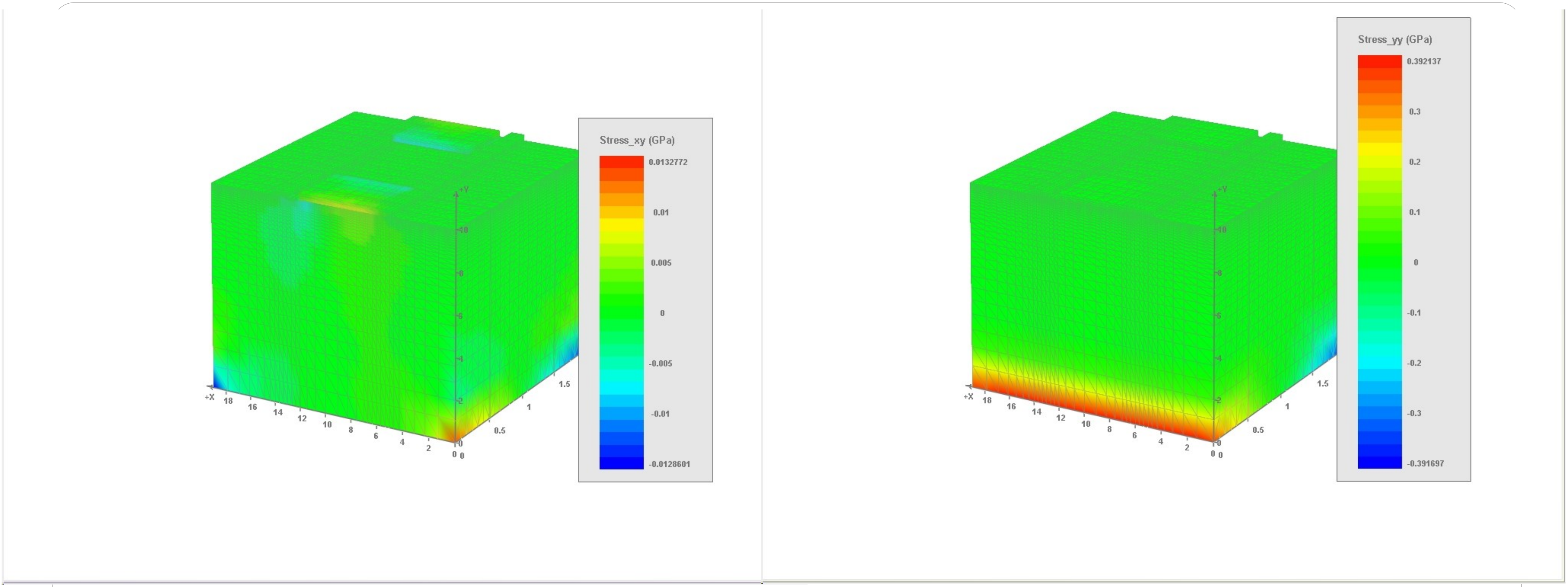
F1:help F2:zoom in F3:zoom out F4:region view F5:rotate F6:move F7:overlay F8:z-connect F9:plot property F10:boundary view F11:full screen F12:mesh view

X=-4.32109e-006, Y=16.6029, Z=1.06213 , Mesh Size = 17152 , Triangle Num = 32032

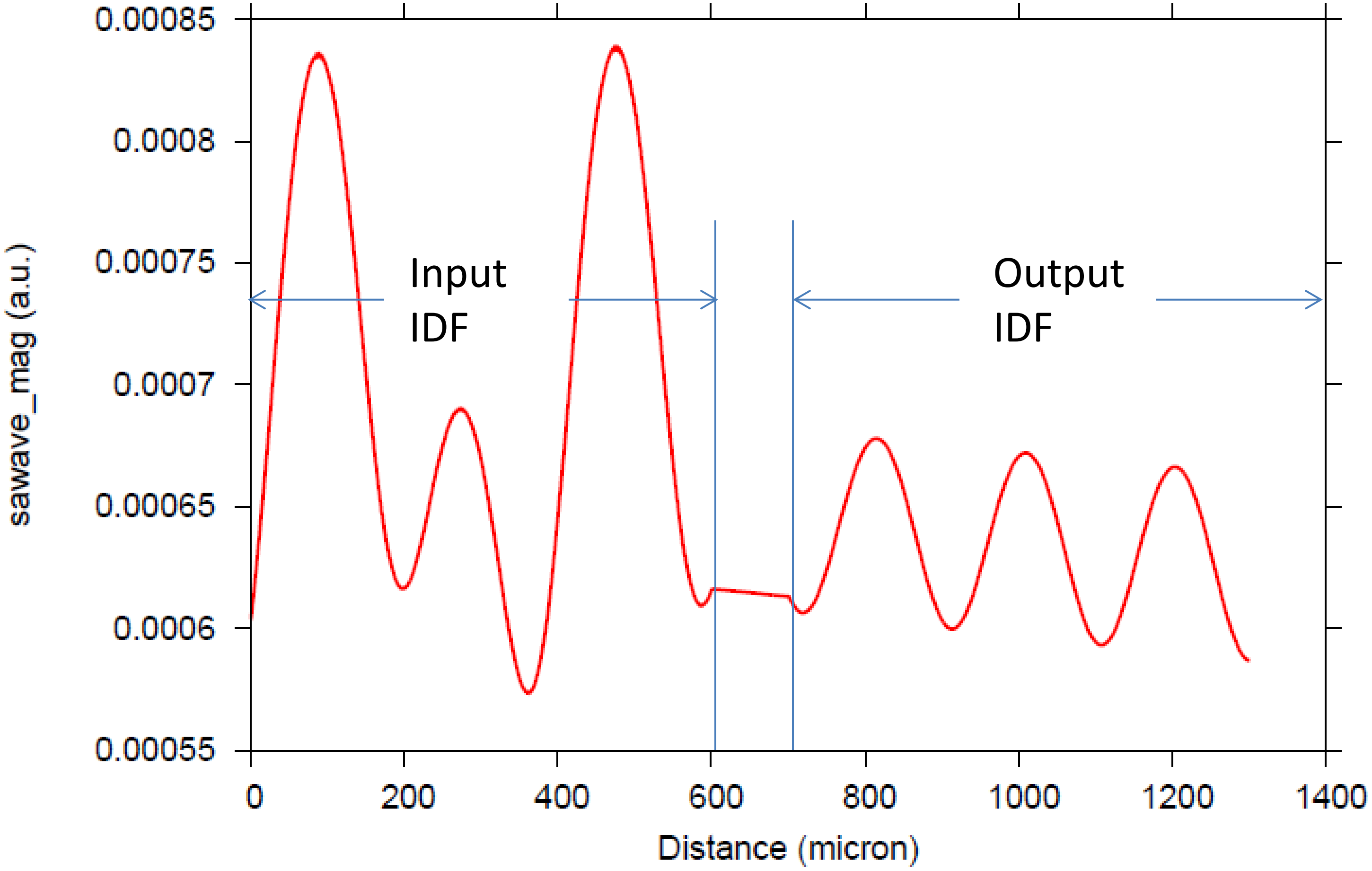
Single period = 2 microns.



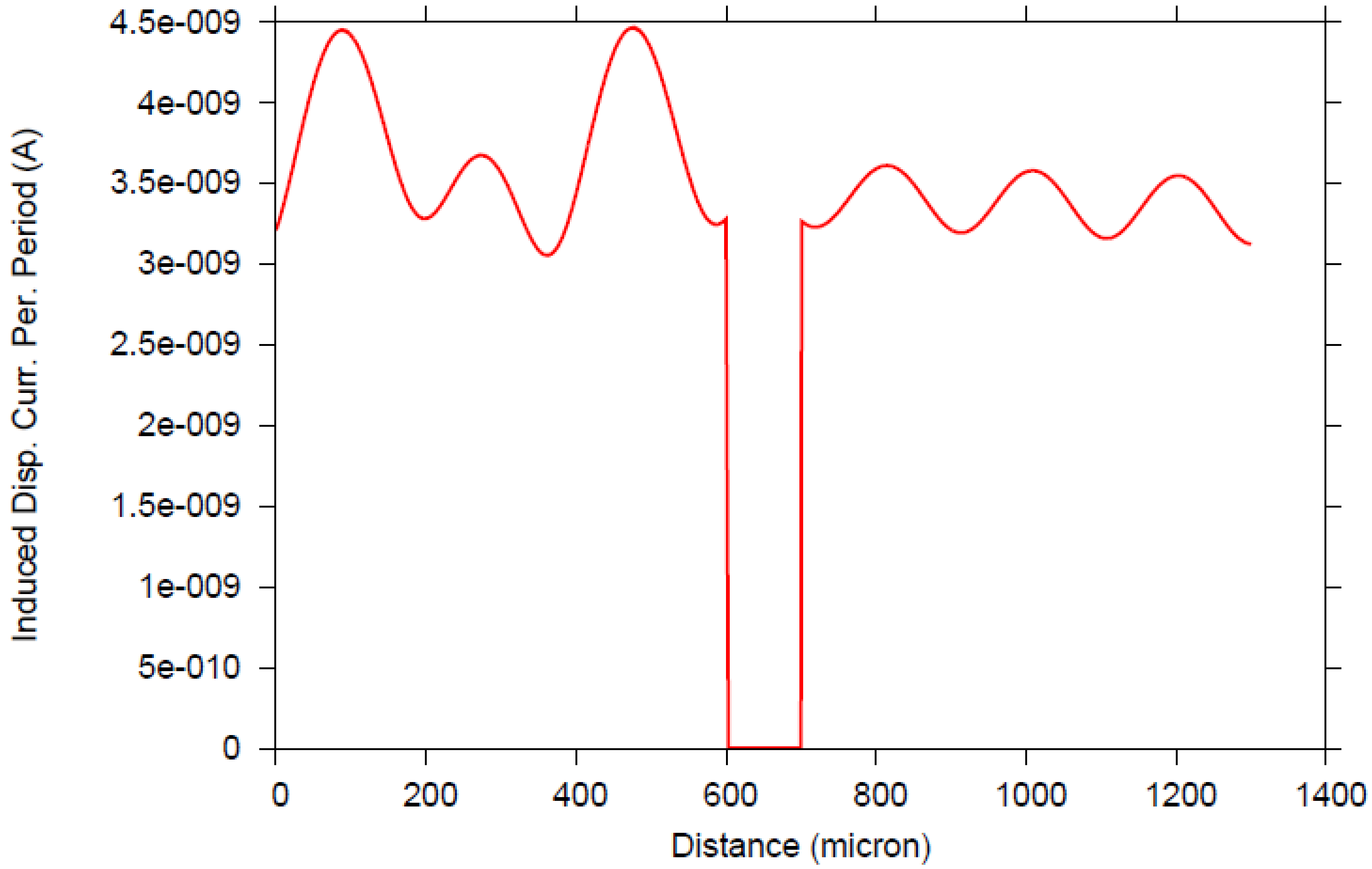
Potential distribution to compute displacement current and also piezo stress source.



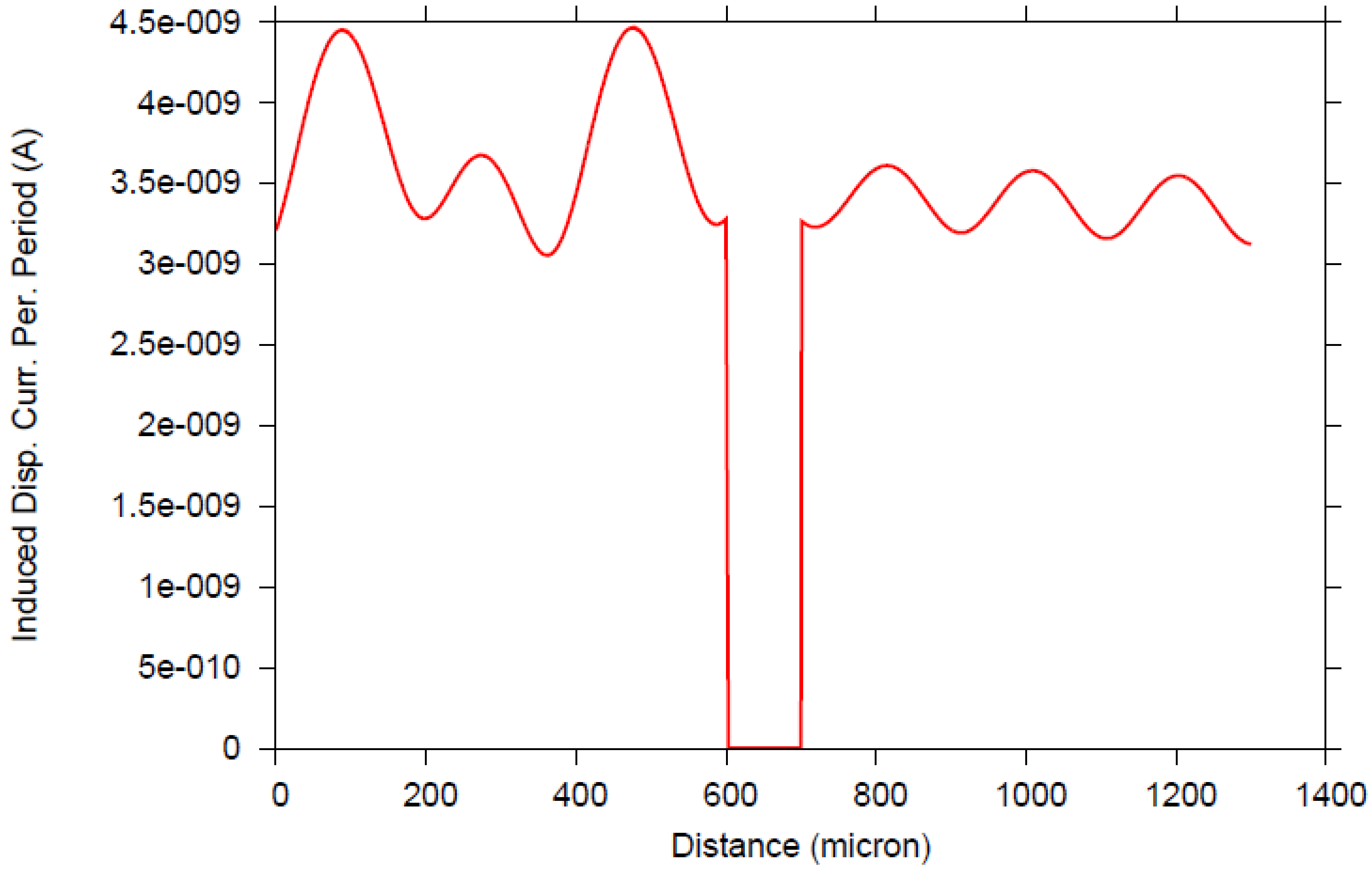
All stress components are computed, but Stress_xy and Stress_yy are used to determined lateral profile of the propagating wave



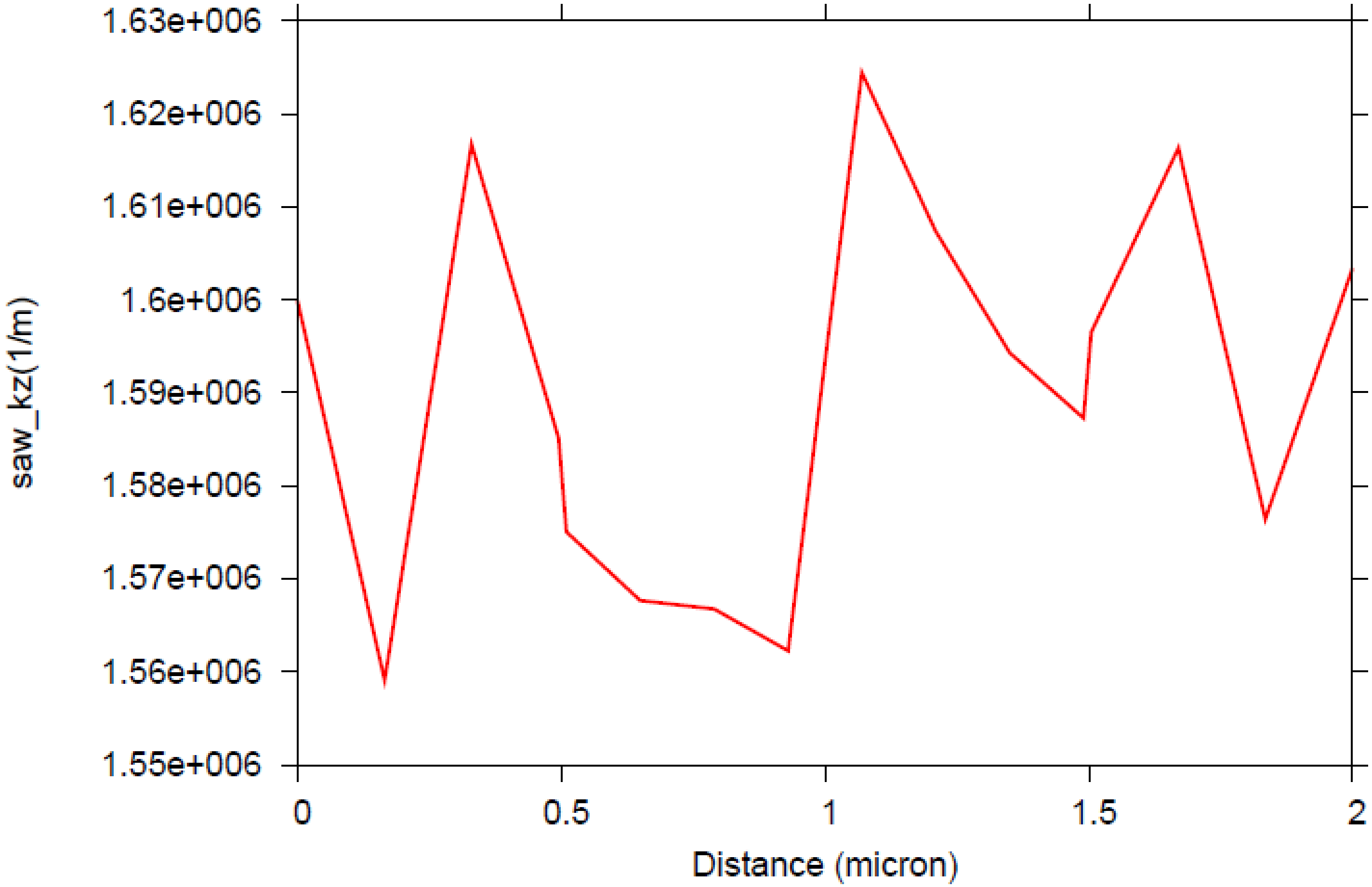
Wave amplitude of SAW from Green's function method at near the Bragg frequency.



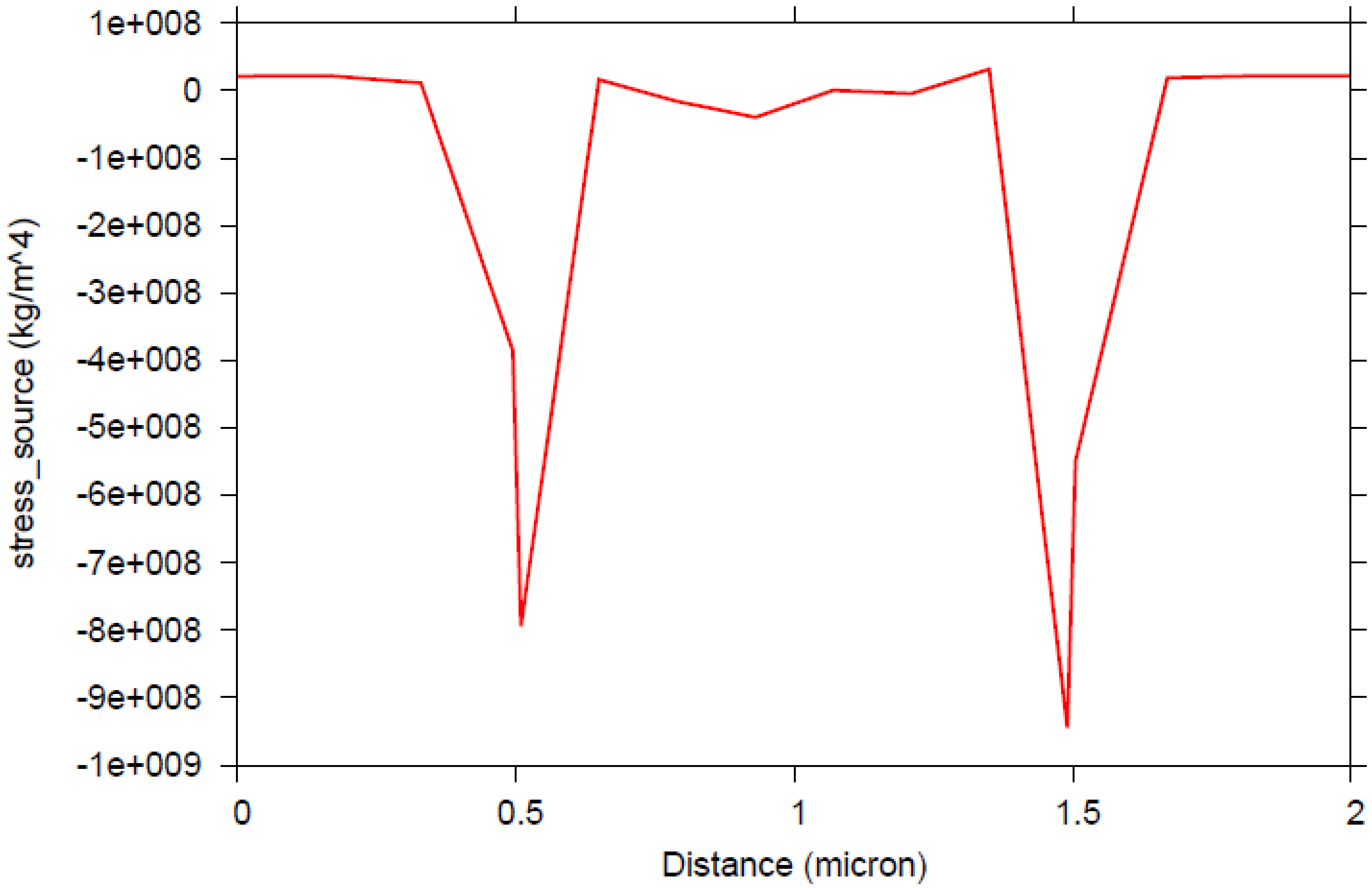
Induced displacement current in IDF per period.



Induced displacement current in IDF per period near Bragg frequency.

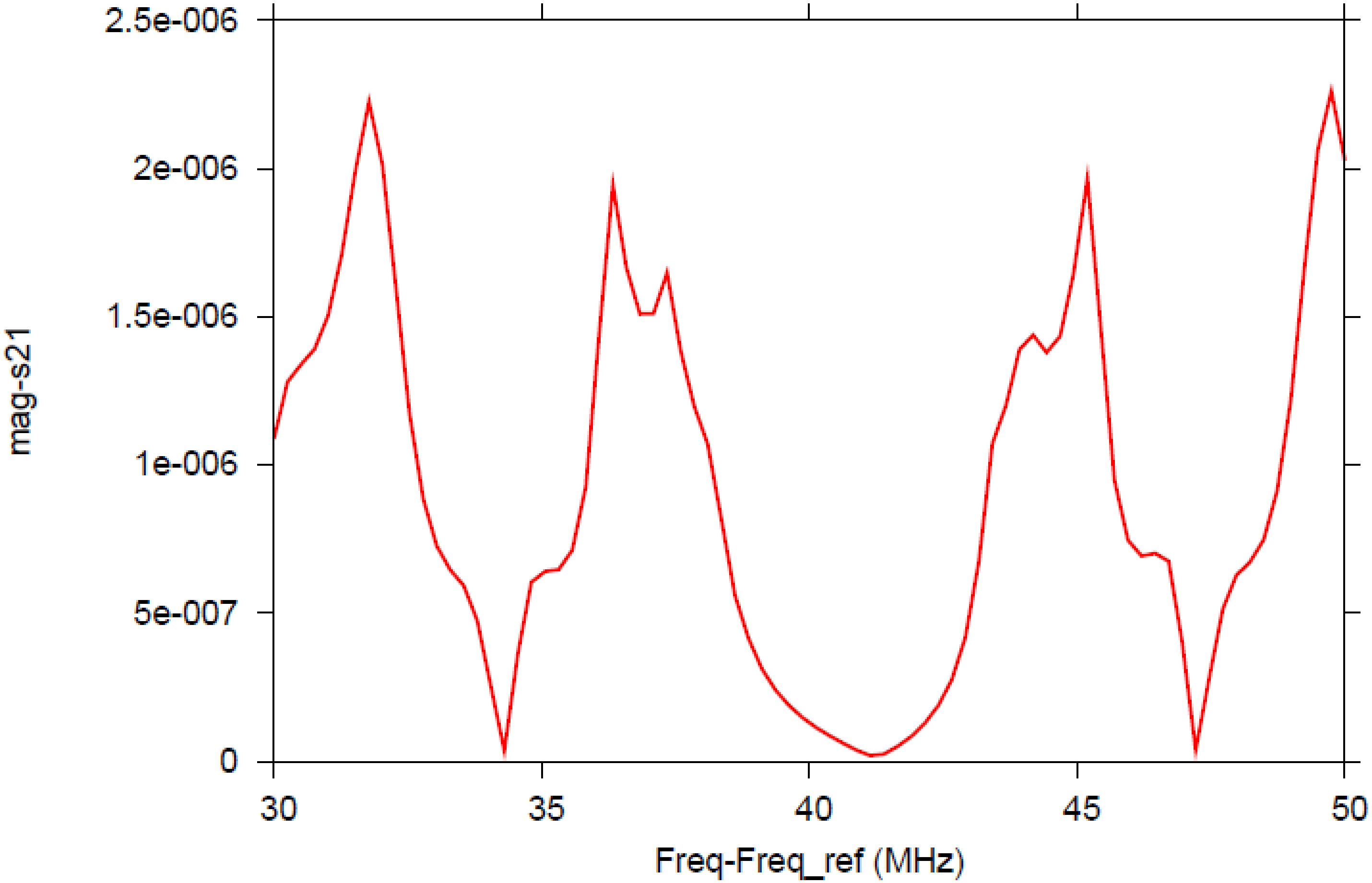


Rayleigh wave vector versus distance. Coupling coefficient kappa is extracted for coupled mode theory.

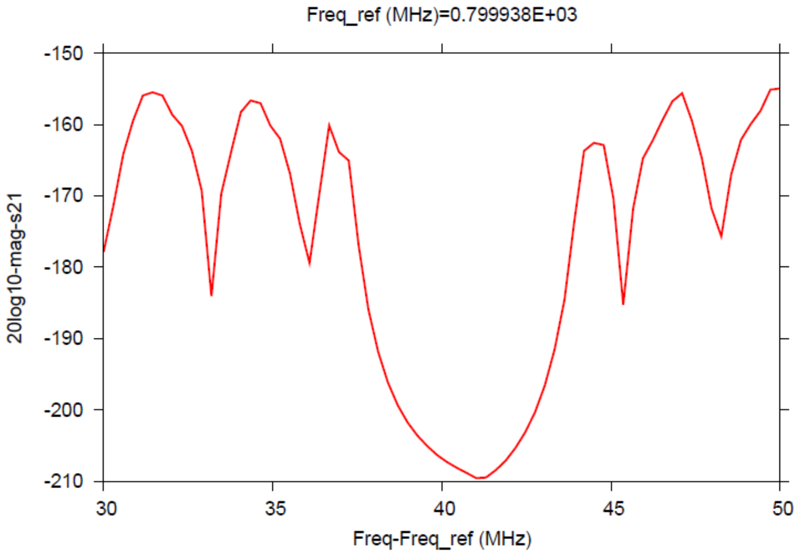


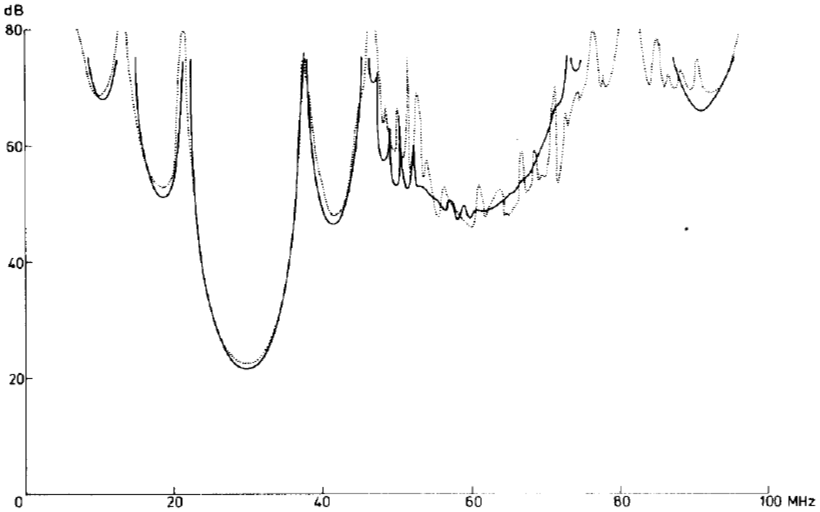
stress source averaged over lateral wave profile, used as source term in Green's function analysis.

S-parameter output



Trend comparison with experiment





Transfer characteristics from 4 IDF of a long SAW device (Quartz/Cu).

4 pair insertion loss measurement on LiNbO3/unknown-metal (Ref: IEEE Trans. Sonics and Ultrasonics, vol. 24, p. 147, 1977)

NovaTCAD

Summary

- For the first time, a specialized 3D SAW device simulator is available commercially.
- High frequency analysis of the whole SAW device can be performed efficiently based on combined 3D stress solver and Rayleigh wave coupled mode solver.
- Advance features include crystal orientation, metal mass loading, open and short circuit effects and all stress component analysis.
- Commonly measured quantities such as S-parameters can be conveniently obtained.

Crosslight Customer Locations

Over 300 customers located around the world

NovaTCAD

A Canadian company with 20 years of history

*The world's **first** commercial TCAD for laser diode*

*The world's **No.1** provider of optics and photonics TCAD*

*The world's **most advanced** stacked planes 3D TCAD*