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Abstract

The following document presents design methodology improvements brought to Coventor tools suite to enable PiezoMEMS devices modelling and improve analyses. It first presents the Process Design Kits implementation in SEMulator3D, CoventorWare and MEMS+. Design Kits are made of Material Database, Process Descriptions specific to each tools and template layouts. Then a second part is dedicated to our latest tool behavioural modelling MEMS+ and the addition of a piezoelectric layer into flexible plates elements to take into account both actuation and sensing behaviour of PiezoMEMS devices. Last part is the description of the electrical circuit option added in the Finite Element mechanical solver MemMech of CoventorWare tool enabling a realistic analysis of piezoelectric sensing which has a direct impact on energy harvesters study.

Public introduction¹

The following document presents design methodology improvements brought to Coventor tools suite to enable PiezoMEMS devices modelling and improve analyses. It first presents the Process Design Kits implementation in SEMulator3D, CoventorWare and MEMS+. Design Kits are made of Material Database, Process Descriptions specific to each tools and template layouts. Then a second part is dedicated to our latest tool behavioural modelling MEMS+ and the addition of a piezoelectric layer into flexible plates elements to take into account both actuation and sensing behaviour of PiezoMEMS devices. Last part is the description of the electrical circuit option added in the Finite Element mechanical solver MemMech of CoventorWare tool enabling a realistic analysis of piezoelectric sensing which has a direct impact on energy harvesters study.

¹ According to Deliverables list in Annex I, all restricted (RE) deliverables will contain an introduction that will be made public through the project WEBSITE

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1 INTRODUCTION

Different tools for the design and modeling of piezoMEMS have been developed and are available. These software tools are calibrated to the PZT processes and enable engineers to simulate and optimize piezoMEMS designs before committing to build-and-test cycles. Coventor's MEMS+ and CoventorWare provide a design and simulation platform for MEMS designers, enabling them to simulate end-product performance specs such as sensitivity, linearity, frequency response, signal-to-noise, and temperature stability. SEMulator3D is a unique modeling tool for virtual fabrication, enabling them to review designs and detect process issues in advance of actual fabrication.

MEMS+™

A behavioral modelling tool which allows quickly exploring design alternatives and optimizing performance at high accuracy. The platform is composed of 3 modules: a material database, a process editor and Innovator which is the 3D builder of the MEMS structure.

The design platform MEMS+ allows to, quickly explore design alternatives, and to optimize performance with high accuracy. With Coventor's design flow the PZT technology comprising material and process data is already defined. To start with, a model of the piezoelectric device is constructed in MEMS+. Here, the MEMS designer works in a 3D graphical environment to assemble a parametric model using high-order MEMS-specific finite elements (piezo-mechanical shells). Each element is linked to the process description and material database so that piezoelectric material properties and electrodes are assigned automatically. The high-order elements give a precise mathematical description of the device physics using a low number of degrees of freedom. This enables rapid, accurate simulation of the device physics in Matlab/Simulink, and the ability to easily co-simulate the device with the conditioning circuit in Cadence Virtuoso. For example, the designer can tune the piezoMEMS device dimensions to attain a maximum actuation displacement or a certain resonance frequency before simulating the device with different electronic circuits to compare the performance of each type.

COVENTORWARE™

A multi-physics field solver based analysis framework (Finite Element and Boundary Element methods) including a materials property database, a process and layout editors, a 3-D model and mesh generator, and field solvers for electrostatics and mechanics, the latter with boundary conditions and features for PiezoMEMS. It includes a process entry user interface with a ready to use library of foundry processes, e.g. MoveMEMS SINTEF process.

For PiezoMEMS device the module of interest is MEMMECH.

Further detailed modelling can be undertaken using CoventorWare's field (or Finite-Element) solvers to investigate details of the design. For example, the design can be checked for high stress areas that may lead to breakage when the device is overloaded due to a shock. Gas damping coefficients can also be simulated and included in the MEMS+ model to accurately predict the Q-factor. An additional benefit is that simulation results from MEMS+ and CoventorWare can be verified against each other. Simulating piezoelectric harmonic analysis with a linear resistive load is one such example of a point of comparison between both tools. Coventor's solution for piezoelectric devices combines MEMS+ and CoventorWare to provide hybrid solution that solves the coupled and multi-domain physics not addressed with traditional point tools.

SEMULATOR3D™

A Virtual Prototyping tool which uses novel "voxel" technology (volumetric pixels) to build highly detailed, virtual prototypes. Input is from 2D masks in industry-standard GDSII format, along with a description of the specific fabrication process.

SEMulator3D offers a productive methodology that enables engineers to understand and communicate process flow and device design through interactive visualization and quantitative measurements. Areas of usage include process documentation, process modeling and optimization, process communications with foundry customers and piezoMEMS design verification prior to actual fabrication.

This report explains all new features and improvements done for enabling and easing piezoMEMS design. They are presented in three parts. The first one describes the implementation of Process Design Kits in each tool. The second one gives an overview of the new Piezoelectric Flexible Plate model added to our existing library of behavioural components included in MEMS+ and its advantages. The third one presents the options added to the standard FEA solver Analyzer to broaden the scope of piezoMEMS devices which can be studied by the solver.

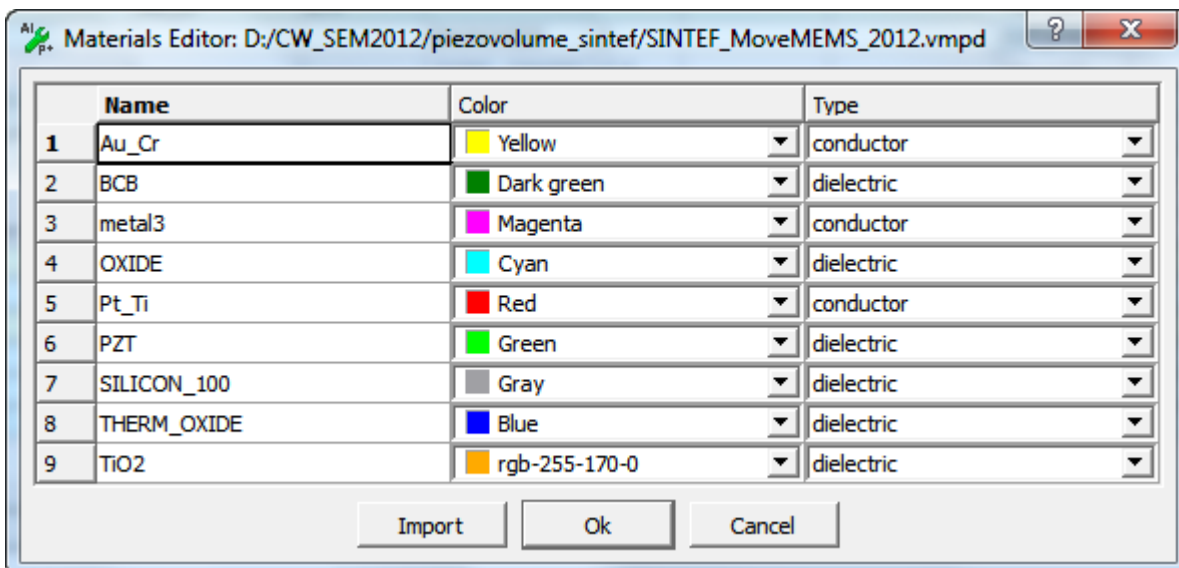
2 PDKS

The three tools MEMS+ (Behavioural Modelling), CoventorWare (Finite Element Modelling), and SEMulator3D (Virtual Prototyping) need technology inputs. A technology is basically described by the materials properties (like PZT or Silicon) and the fabrication process (stack of deposition and etch of layers). Depending on the tool, you'll need different data and level of accuracy in the description. The first paragraph starts describing what has been done to update the SINTEF MoveMEMS Material Database. Then the second paragraph is a summary of implementation of MoveMEMS process in all tools.

2.1 Material Databases

2.1.1 Virtual Prototyping

SEMulator3D is a fabrication emulating tool. It requires only material names, type (conductor or dielectric) and colours. Figure 2.1 shows the MoveMEMS SEMulator3D material database (.vmpd file content) which is attached to the process description file. This can be checked in the file properties.



	Name	Color	Type
1	Au_Cr	Yellow	conductor
2	BCB	Dark green	dielectric
3	metal3	Magenta	conductor
4	OXIDE	Cyan	dielectric
5	Pt_Ti	Red	conductor
6	PZT	Green	dielectric
7	SILICON_100	Gray	dielectric
8	THERM_OXIDE	Blue	dielectric
9	TiO2	rgb-255-170-0	dielectric

Figure 2.1 SEMulator3D Material Database

2.1.2 Behavioral and Finite Element Modeling

MEMS+ and CoventorWare require the physical materials properties (electrical, mechanical, thermal and piezoelectric) to simulate piezoMEMS devices operation. The following values in table 2.1 have been integrated into both tools.

Note: TiO2 has not been used because it is a very thin oxide (100nm) under PZT only used for process A. It can be neglected for simulations. Yet if it is required its properties are to be provided by SINTEF.

Properties	SILICON_100	OXIDE	THERM_OXIDE	PZT	Au-Cr	Au-TiW metal3 or top electrode	Pt-Ti	BCB passivation layer
Young Modulus	cubic: $E_x=E_y=E_z=130.18$ GPa			$C_{xxx}=C_{yyy}=132$ GPa				
	$C_y=C_x=C_z=79.6$ GPa	70 GPa	70 GPa	$C_{xyy}=71$ GPa	78 GPa	78 GPa	168 GPa	2.9 Gpa
	wafer 100 oriented			$C_{zzz}=115$ GPa				
				$C_{yxy}=C_{zyz}=26$ GPa				
Poisson ratio	$V_{xy}=V_{yz}=V_{yx}=0.278$	0.3	0.3	$C_{yyy}=30$ GPa	0.35	0.35	0.35	0.34
Density	2331 kg/m ³	2220 kg/m ³	2220 kg/m ³	7750 kg/m ³	19300 kg/m ³	19300 kg/m ³	21450 kg/m ³	1050
Residual Stress	0	-300 MPa	-300 MPa	175 MPa	282 MPa	282 MPa	700 MPa	-0.1xT+57.315 28 MPa at 293.15K
Thermal Coef. of Expansion zero stress Temp. -293.15K	2.49e-6 /K	5e-7/K	5e-7/K	2.5e-6 /K	1.39622e-5 /K	1.39622e-5 /K	8.86349e-6 /K	4.194e-5 /K
Thermal conductivity	157 W/(m*K)	1.4226 W/(m*K)	1.4226 W/(m*K)	1.5 W/(m*K)	297 W/(m*K)	297 W/(m*K)	71.6 W/(m*K)	7.381e-4*T+7.418e-2 0.294 W/(m*K) at 297.15 K
Specific heat	703 J/(kg*K)	1000J/(kg*K)	1000J/(kg*K)	0	128.7 J/(kg*K)	128.7 J/(kg*K)	133 J/(kg*K)	1.27e-7*T+4.71e-6
Electrical conductivity	1400 S/m	1e-10 S/m	1e-10 S/m	2.5e-7 S/m	4.4e7 S/m	4.4e7 S/m	1e7 S/m	1e-17 S/m
Permittivity	0	3.9	3.9	$\epsilon_{xx}=\epsilon_{yy}=\epsilon_{zz}=1600$	0	0	0	2.65
Piezoelectric coefficients	-	-	-	$e_{xxz}=e_{yyz}=10.5$ C/m ² $e_{zxx}=e_{zyy}=-4.1$ C/m ² $e_{zzz}=14.1$ C/m ²	-	-	-	-

Table 2.1: Material database

In Coventorware the technology is set in the model builder by browsing the corresponding files in the Build Solid Model window. Materials (.mpd file), process (.proc) and layout inputs are required to build the 3D meshed model necessary for mechanical and piezoelectric analyses. The Material Database is shown in Figure 2.2.

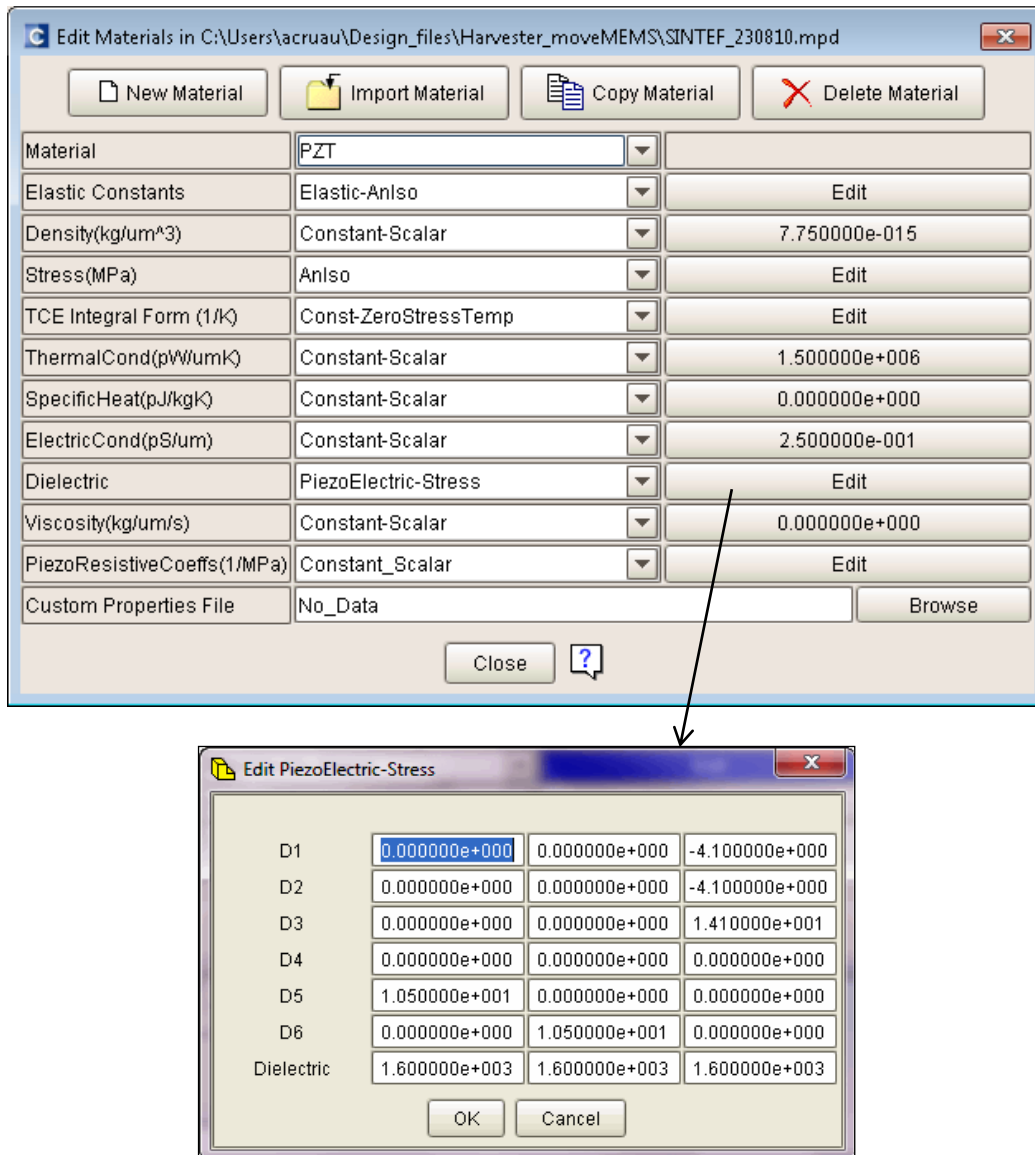
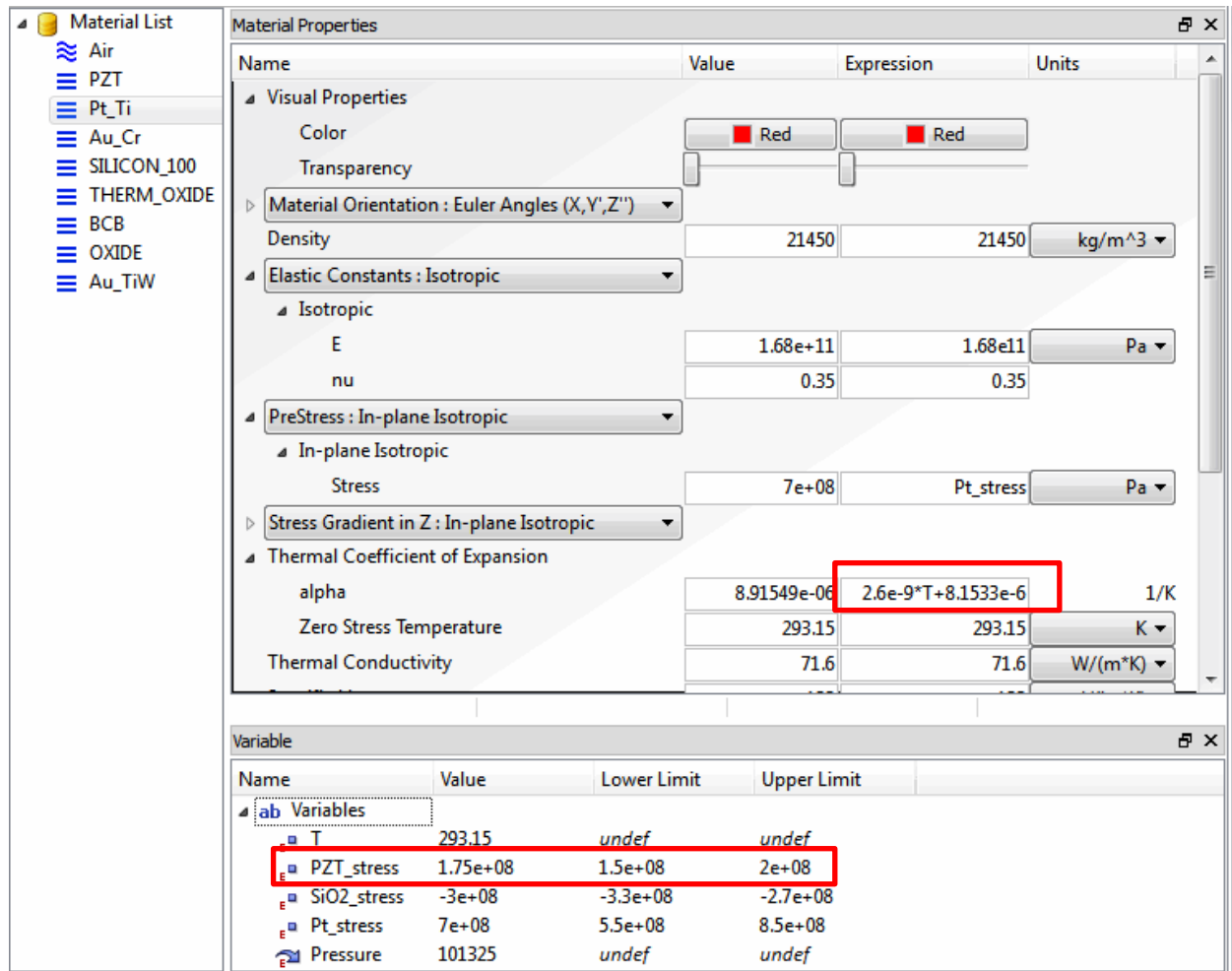


Figure 2.2 CoventorWare MPD for SINTEF showing PZT properties

MEMS+ tool allows more flexibility in the Material Database. It can include statistical data (distribution, limits, ...) as can be seen in Figure 2.3. All material and process step properties (such as Modulus of elasticity, layer thicknesses, side-wall angles etc.) can be defined as absolute values, variables or algebraic equations. A combination of variables and algebraic equations allows for properties to be mutually dependent on other properties, environmental variables (e.g. temperature and humidity) or even entirely abstract variables such as the equipment settings of a given fabrication process.



Name	Value	Expression	Units
Visual Properties			
Color	Red	Red	
Transparency			
Material Orientation : Euler Angles (X,Y,Z")			
Density	21450	21450	kg/m ³
Elastic Constants : Isotropic			
Isotropic			
E	1.68e+11	1.68e+11	Pa
nu	0.35	0.35	
PreStress : In-plane Isotropic			
In-plane Isotropic			
Stress	7e+08	Pt_stress	Pa
Stress Gradient in Z : In-plane Isotropic			
Thermal Coefficient of Expansion			
alpha	8.91549e-06	2.6e-9*T+8.1533e-6	1/K
Zero Stress Temperature	293.15	293.15	K
Thermal Conductivity	71.6	71.6	W/(m*K)

Name	Value	Lower Limit	Upper Limit
Variables			
T	293.15	undef	undef
PZT_stress	1.75e+08	1.5e+08	2e+08
SiO2_stress	-3e+08	-3.3e+08	-2.7e+08
Pt_stress	7e+08	5.5e+08	8.5e+08
Pressure	101325	undef	undef

Figure 2.3: Material database for MoveMEMS in MEMS+

The MEMS+ design environment for PDK gives the foundry full control over which variables are to be exposed (and so transferred and controllable) to the process editor.

2.2 Process Descriptions

Once materials set the next step is to define the clean room process using those materials to create PiezoMEMS devices.

2.2.1 Virtual Prototyping

The description for SEMulator3D should be detailed enough to obtain a highly realistic-looking device or chip. More steps and more options are available to reach that aim. All steps of the GUI (General User Interface) correspond to a python function and the complete process is scriptable and can be run as a text file in a shell command. Figure 2.4 shows the process file created.

Number	Step Name	Material Name	Thickness	Mask Name	Depth	Mask Offset	Sidewall Angle	Comments
0	Wafer Setup	SILICON_100	500	SubstrateMask				
1	SOI							Add to Start wafer to create SOI...
1.1	Buried Oxide	OXIDE	0.5					
1.2	Crystal Silicon	SILICON_100	8					
2	Front and Back Oxidation		1.5					the device layer of 8 microns will t...
3	Sputter TiO2 (option A)	TiO2	0.4					Chemical Solution Deposition (CS...
4	Sputter Bottom Electrode (option B or C)	Pt_Ti	0.4					Note: thickness is around 120nm....
5	PZT Deposit	PZT	2					CSD
6	Top electrode Deposit	Au_Cr	0.4					TIW can also be chosen for adhes...
7	Backside Etch Mask patterning			BACKOXIDE	2			RIE(anisotropy 0) or wet etch wit...
8	Top electrode patterning (option A)			TOPEL_FINGER	0.4			photolithography and wet etch
9	Top electrode patterning (option B or C)			TOPEL	0.4			photolithography and wet etch
10	Piezoelectric Layer Patterning (option B or C)			NOPIE	2			
11	Pattern Bottom Electrode (option C)			BOTEL-NOPT	0.4			
12	Passivation and metal pads (option A)							
13	Passivation and metal pads (option C)							
13.1	Passivation layer deposit	BCB	10					used as a passivation layer
13.2	Passivation etch			DIELOPEN				
13.3	Deposit metal3	metal3	0.7					NiCr/Au is preferred. Cr/Au an alt...
13.4	Metal3 pads patterning			METAL3	0.7			
14	Backside DRIE			BETCH	501			
15	Frontside Release Etch			FETCH	20			

Figure 2.4 SEMulator3D SINTEF MoveMEMS process with C variant enabled.

2.2.2 Behavioral Modeling and Finite Element Modeling

CoventorWare process editor looks like SEMulator3D except only five basic operations (three deposits and two etches) can be combined to create the 3D solid. The aim here is to obtain a meshed model, consequently the device shape is optimized for simulation by simplifying the geometry. An option for rounding corners is available to improve the final device. It is not used in the SINTEF process but can be added by the user.

Number	Step Name	Layer Name	Material Name	Thickness	Mask Name	Photoresist
0	Substrate	Substrate_wafer	SILICON_100	500		
1	Silicon-On-Insulator (SOI)					
1.1	Buried oxide	Buried_Oxide	OXIDE	0.5		
1.2	Crystal Silicon	Si_Handle	SILICON_100	7.4		
2	Wet Oxidation	Oxide_layer	THERM_OXIDE	1.5		
3	Sputtering Bottom Electrode	Bottom_electrode	Pt_Ti	0.16		
4	PZT Chemical Solution Deposition	PZT_piezoelectric	PZT	2		
5	Top Electrode Deposition	Top_electrode	Au_Cr	0.18		
6	Oxide Etch Backside				BACKOXIDE	-
7	Top Electrode Patterning				TOPEL	+
8	PZT patterning				NOPIE	-
9	bottom electrode patterning, passivation and metal pads (option C)					
9.1	Bottom Electrode Patterning				BOTEL-NOPT	-
9.2	Passivation	Passive	BCB	10		
9.3	Openings				DIELOPEN	+
9.4	Pad metalization	Metal3	Au_TIW	0.71		
9.5	Straight Cut				METAL3	+
10	Backside DRIE				BETCH	-
11	RIE Release Etch				FETCH	-

Figure 2.5 CoventorWare SINTEF MoveMEMS process

MEMS+ process editor is used as in CoventorWare to give the 3rd dimension (extrude direction of process) to the device. It needs only the thickness and relative position of layers in the stack. The same three basic deposit operations and two etch ones are available but it means only a z initial position for layers middles and their thicknesses. The etch steps with masks names (names given from MoveMEMS DRM) are also implemented directly after the deposit of the layer so the order is slightly different than what has been done for CoventorWare.

Name	Layer Name	Material Name	Mate	Thickness	Mask Name	Photoresist	Mask Offset	Sidewall Angle
Substrate	Substrate_wafer	SILICON_100		500	GND			
SOI								
SOI oxide	buried_oxide	OXIDE		0.5				
SOI crystal silicon	Si_handle	SILICON_100		7.4				
oxidation	SiO2	THERM_OXIDE		1.5				
PtTi bottom electrode	bottom_elec	Pt_Ti		0.12				
PZT Chemical Solution Deposition	piezo	PZT		2				
AuCr top electrode	top_elec	Au_Cr		0.16				
top electrode patterning					TOPEL	Negative	0	0
PZT patterning					NOPIE	Negative	0	0
bottom electrode patterning					BOTEL_NOPT	Negative	0	0
Conformal Shell1	passivation	BCB		10				
Straight Cut1					DIELOPEN	Positive	0	0
Stack Material1	metal3	Au_TiW		0.71				
Straight Cut2					METAL3	Positive	0	0
back etch					BETCH	Negative	0	0
frontside release					FETCH	Negative	0	0

Figure 2.6 MEMS+ SINTEF MoveMEMS process

The GDS numbers of layout layers will also be added in future MEMS+3 release. These numbers are subject to change and users should ask SINTEF for an update on the technology before using the PDK.

2.3 Layout template

For SEMulator3D, layout templates (one for process B and C and one for process A as SINTEF used during the project) are necessary to translate GDS file into .cat format. This is to link the GDS numbers to layer names.

Some devices are also included like the ones of Figure 2.7.

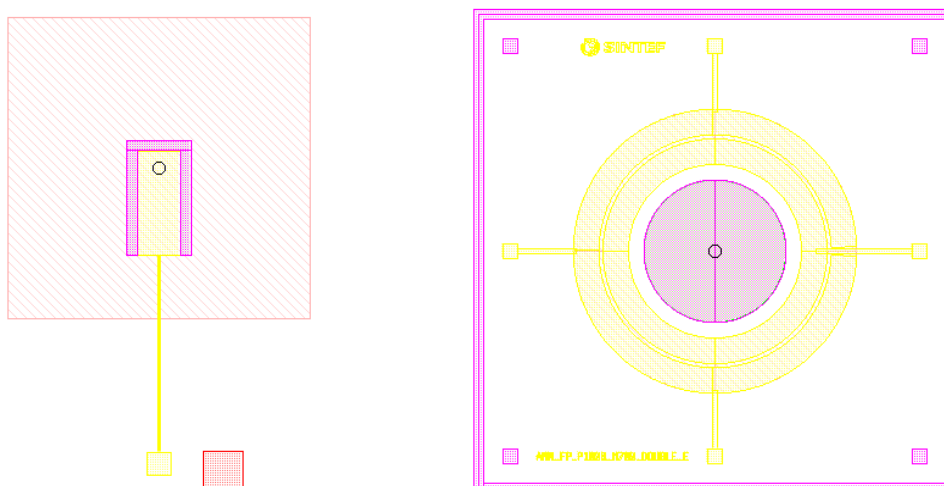


Figure 2.7 Cantilever and piston mirror device layout (see D5.6).

2.4 Conclusion

The PDKs for MoveMEMS technology the MPD and process may be updated with SINTEF inputs. For example, the improvements achieved in the project will be integrated to an up-to-date version of this kit at the end of the project.

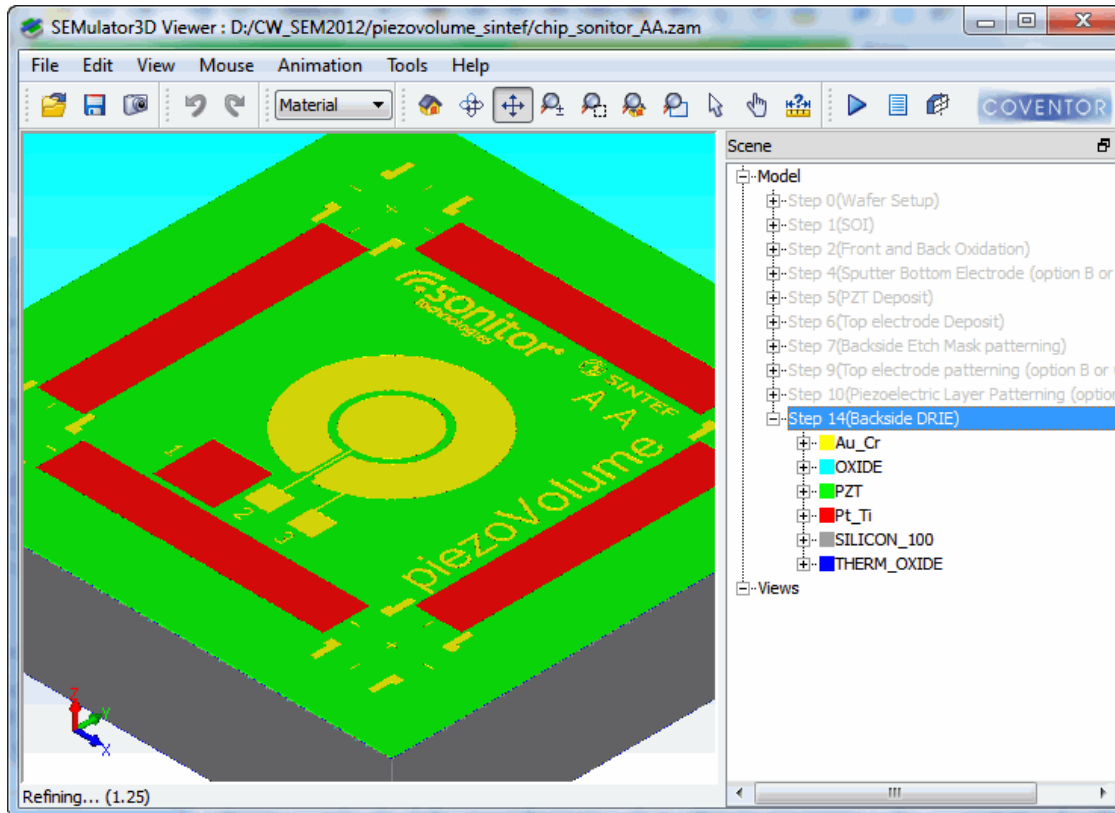


Figure 2.8 Sonitor device emulated with SEMulator3D

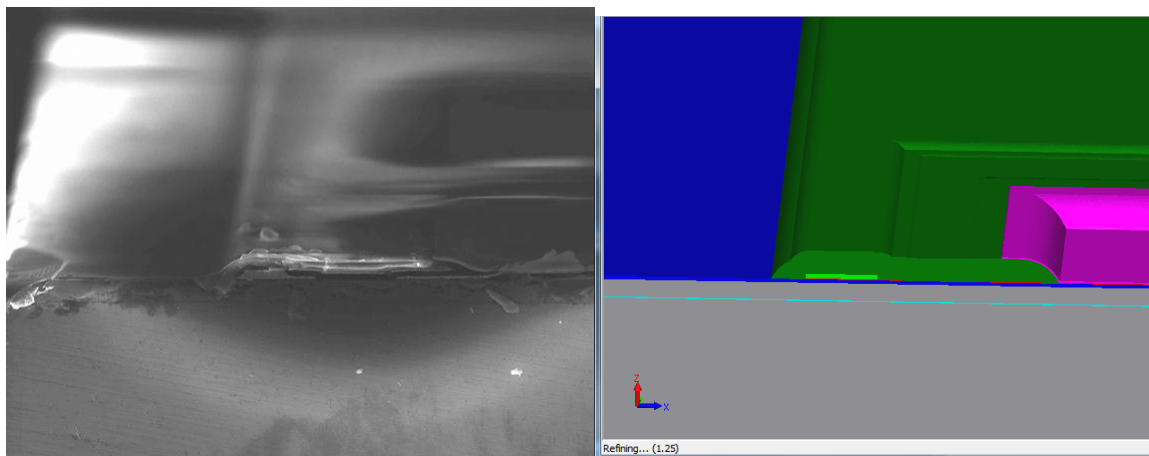


Figure 2.9 Comparison between SEM photo and SEMulator3D emulation

3 PARAMETRIC LIBRARY IMPROVEMENT: PIEZOELECTRIC SHELL

3.1 Shell element model

This component is part of MEMS+ library. It can be combined with other components to build a MEMS structure as in Figure 3.1.

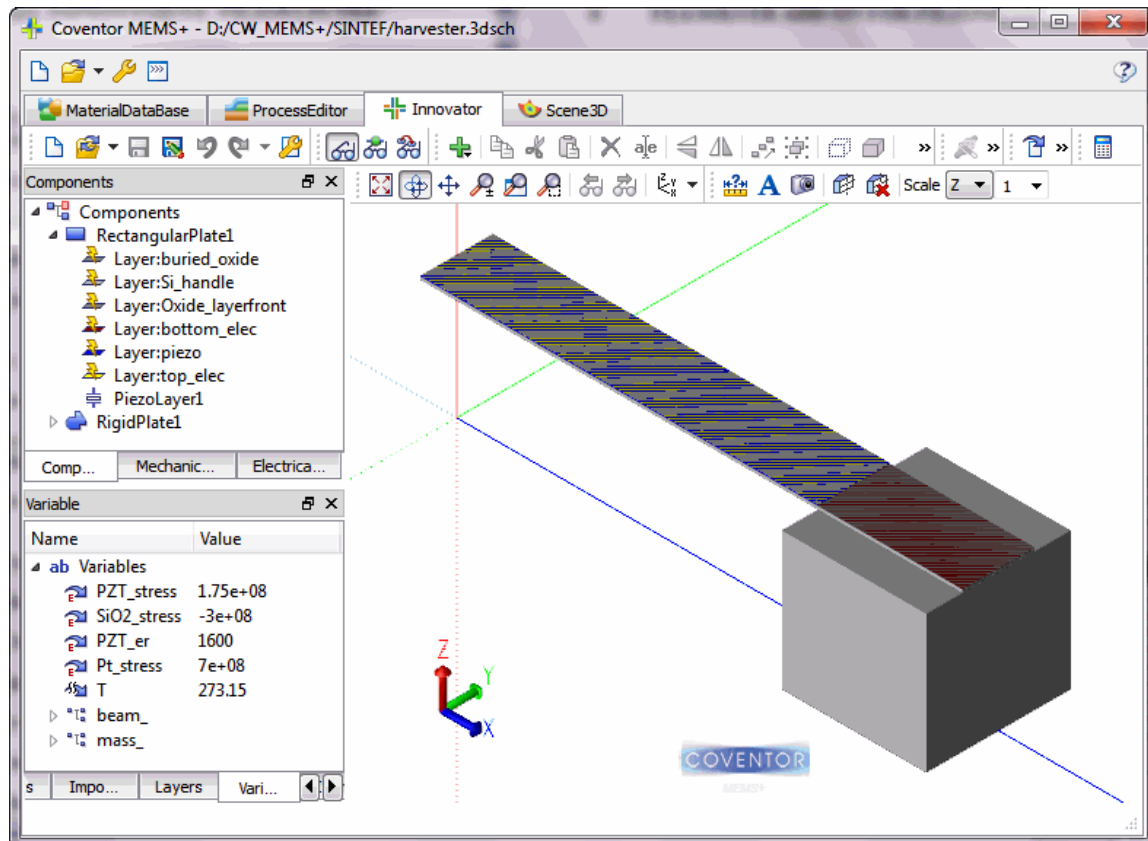


Figure 3.1 MEMS+ device modeling example

The individual material layers of the plates are modeled by a state-of-the-art, nonlinear finite element based on the mixed interpolation of tensorial components approach (MITC). The core functionality of the underlying code is derived from a finite shell element (MITCn) written by Dominique Chapelle and Marina Vidrascu at INRIA ("Institut National de Recherche en Informatique et en Automatique, France"). Refer to *The Finite Element Analysis of Shells: Fundamentals*, Springer, 2003, D. Chapelle, and K. J. Bathe. For an in-depth and detailed explanation of the underlying mathematical model of the used MITCn element. A few fundamental assumptions are summarized below:

- The stress through the thickness of the plate/shell is zero.
- The MITC elements are based on the theory of plates with transverse shear deformations. This theory, developed by E. Reissner and R. D. Mindlin, uses the assumption that particles of the plate originally on the straight line that is normal to the undeformed middle surface remain on a straight line during deformation, but this line is not necessarily normal to the deformed middle surface. The flexible plate elements are capable of handling shear stress.

- The plates have two parameters for specifying order of the polynomial, and the underlying isoparametric finite element formulation expresses element coordinates and element displacements in the form of interpolations using the natural coordinate system of the element. The higher-order elements shows a significantly more accurate bending behavior, which comes at the price of larger simulation time resulting from the additional degrees of freedom (DOFs) used for the Interpolation.

3.2 Adding the piezoelectric effect

To add a piezoelectric layer you need first to use in the stack a material from the Material Database which has a piezoelectric coefficient matrix e . Then on a flexible plate (rectangular or other shapes) you right click to add a Piezoelectric Layer. Once added, top and bottom electrodes appear as Electrical connectors named E1 and E2 by default (if no other electrical connectors have been added prior to that step).

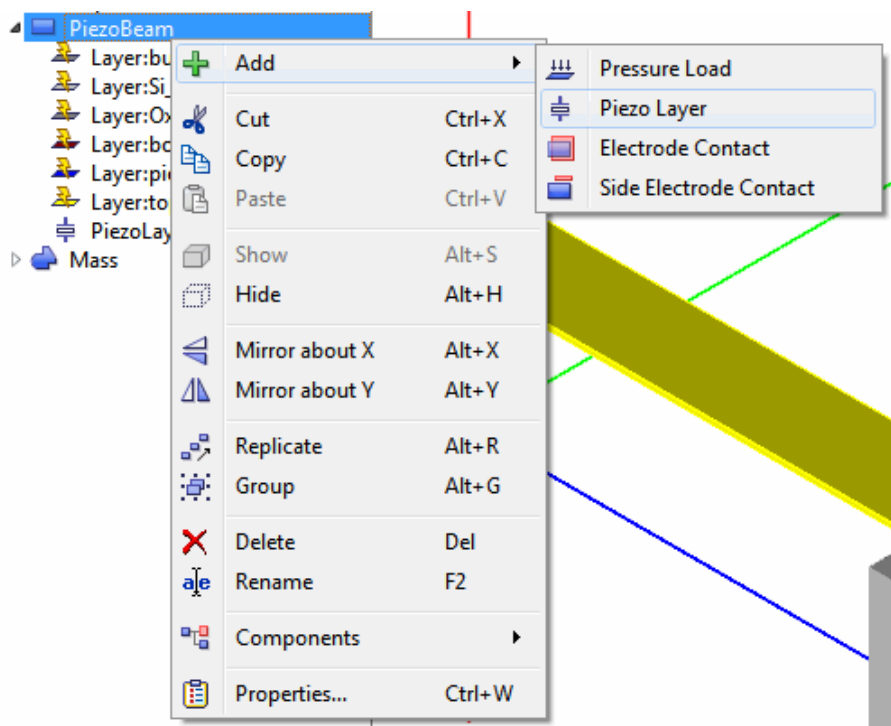


Figure 3.2 How to add a piezolayer in MEMS+ flexible plates.

During the simulation, a voltage-dependent piezoelectric stress σ_p is applied to the PZE layer: $\sigma_p = -eE$, where E is the electric field vector in the PZE layer : $E = E_z = (V_{bottom} - V_{top}) / h$ h is the thickness of the piezoelectric layer, and $(V_{bottom} - V_{top})$ is the voltage difference applied between the two electrical pins E1 and E2.

The built-in PZE layer model can also be used for piezoelectric sensing. Piezoelectric sensing is modeled by creating a stress/strain-dependent current flow between the element pins. The total current i , including the electrical current generated by the internal resistance $1/\rho$, the capacitance cap and the PZE layer strain depending charge Q is calculated as follows:

$$i = \frac{d}{dt}(V_t - V_b)cap + \frac{dQ}{dt} + (V_t - V_b)\rho$$

4 FEA SOLVER ADD-ON FOR PIEZOMEMS

4.1 Description

PiezoMEMS devices typically exist within a larger electrical circuit. In some cases, the mechanical simulation of the MEMS device requires modeling all or part of this larger circuit. The new option enables harmonic analyses of piezoMEMS device including simple circuit elements, such as resistors, inductors, and capacitors.

Two typical applications for this circuit element capability are

- Energy harvesters, where vibration produces electrical current to other components in the circuit.
- Active damping, where patches of piezoelectric material are added to a larger mechanical structure to control its vibration. As the structure vibrates, current is produced by the piezoelectric material and directed to a resistor in the circuit. The resistor converts part of this current to heat, thus dissipating the motion.

In CoventorWare tool you need to use MemMECH module for new analysis and set the Piezoelectric physics and the Direct Harmonic Additional Analysis, then Circuit Elements boundary conditions appears in the menu. Three components are available to build a small circuit: resistor, capacitor, or inductor. They are attached to two terminals, denoted Terminal_1 and Terminal_2, which are surfaces with potential, floating conductor or electrical_node boundary conditions are defined.

An Electrical_Node is simply a new circuit node added to the model to which additional circuit elements can be attached; this allows the creation of simple RLC circuits.

These Electrical_Nodes are implicit; they are not actual entities in the solid model.

When one or more resistors are included in the model, electrical current is converted to heat and dissipated from the model. As mentioned above, this typically damps the motion of the structure.

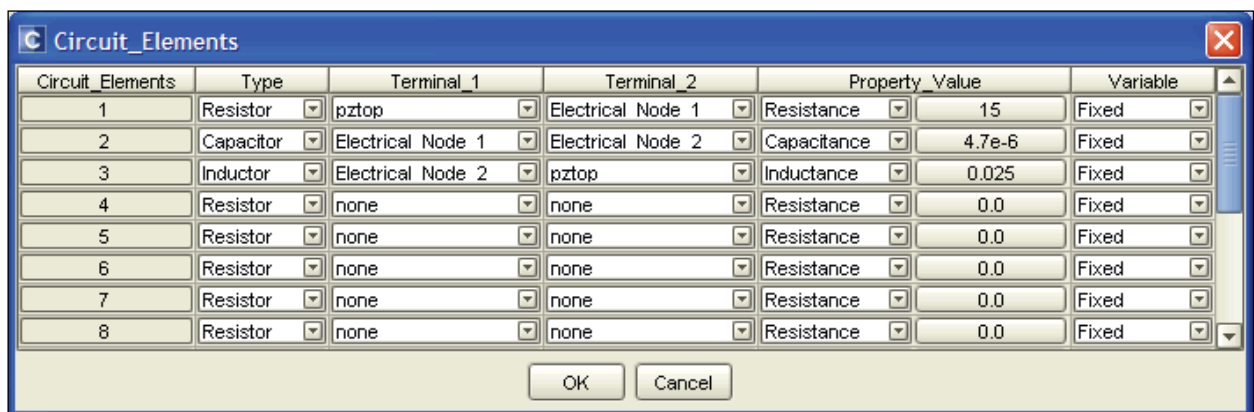


Figure 4.1: New Circuit Element Boundary Conditions

The circuit element applications described above usually do not include active electrical elements. However, it is possible to include an active AC voltage source in a MemMech analysis by defining an extra block of piezoelectric material that is fixed to prevent motion and has a fixed potential on one electrode and an harmonic potential on the counter electrode surrounding the piezoelectric layer. The desired electrical potential is prescribed on the counter electrode. This approach can be used to verify a circuit model before including it in the larger electromechanical simulation.

The main results obtained from this simulation are the amount of energy dissipated the amount of damping resulting from this current dissipation (Quality Factors menu). Other results include currents, power and node potentials.

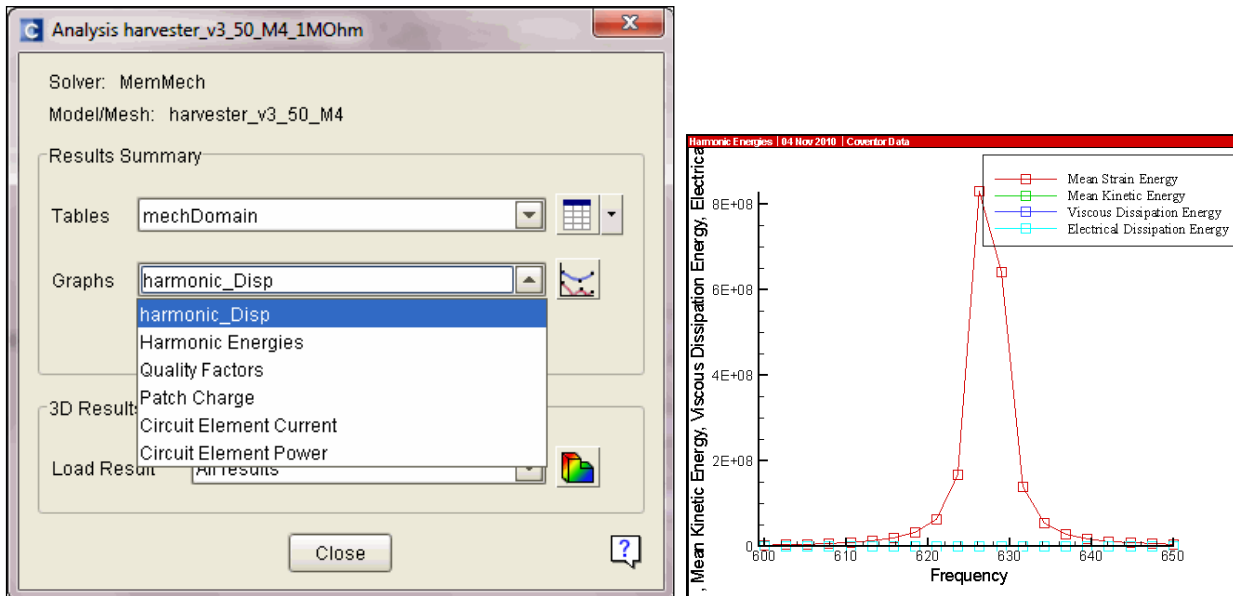


Figure 4.2 Results Window and example graph

4.2 Extra Material

To support people using this new option we have added an application note to the explanation given above. It is part of the document called CoventorWare Application Notes as section2: “Modeling Circuit Elements for PZE Analysis”. This document is included in the installation folder. This note examine a simplified energy scavenger analyzed in "A Distributed Parameter Electromechanical Model for Cantilevered Piezoelectric Energy Harvesters," Erturk, A. and D. J. Inman, Journal of Vibration and Acoustics, 130, 4, August 2008. Results from MemMech are compared with the analytical results, and it is shown that all both methods predict similar mechanical and electrical behavior for this device.

Deliverable 5.6 will contain more application notes on using our tools for piezoMEMS devices.

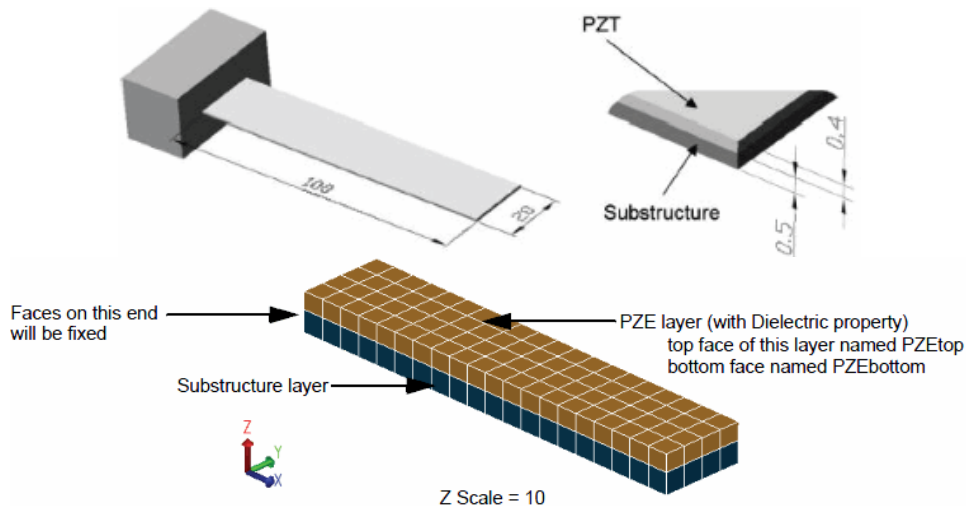


Figure 4.3 Application Note Energy harvester device

5 CONCLUSION

All improvements presented in paragraphs 3 and 4 have been integrated into tools which have been released this CoventorWare and MEMS+. The PDKs are available on request and will be integrated in the software. They may be updated with SINTEF's input and agreement. The deliverable 5.6 will present the PiezoMEMS devices studied with Coventor tools.