Electric Field in Thin Films

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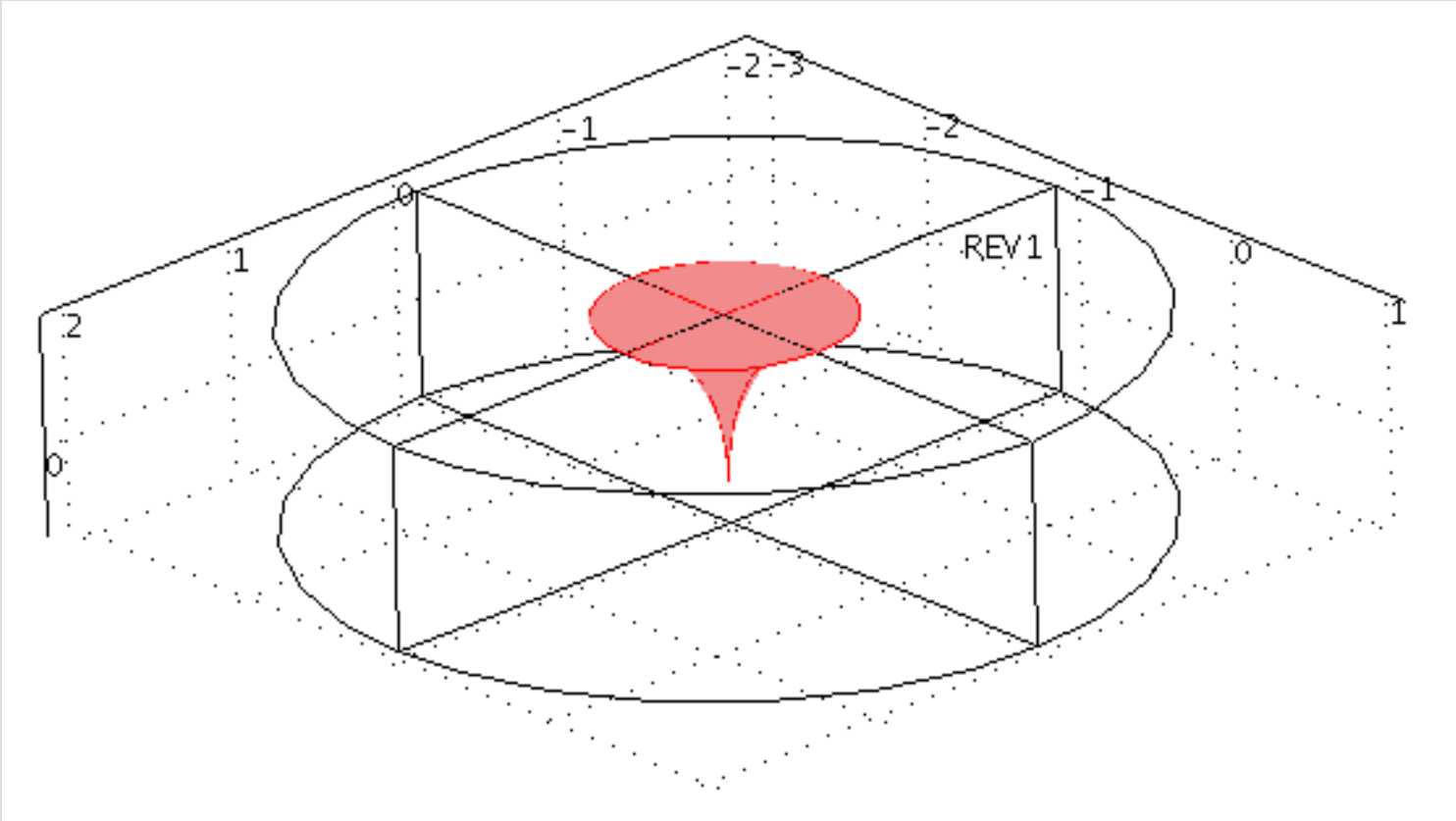
Motivation

- thin films of silicon are used in solar cells
- AFM is used to probe the structure
- we want quantitative interpretation of the results

Geometry



microcrystalline grain (red) and amorphous silicon (the rest)

Electronic Transport

- equation:

$$\nabla \cdot \sigma \nabla \phi = 0$$

$\sigma(x, y, z)$ ... conductivity

$\phi(x, y, z)$ ... electric potential

Gmsh

- http://www.geuz.org/gmsh/
- opensource
- an automatic 3D finite element grid generator
- build-in CAD engine
- parametric input
- post-processor, advanced visualization capabilities

- in my experience superior to femlab

Geometry

t4.geo (~/femlab/grain1) - gedit

File Edit View Search Tools Documents Help

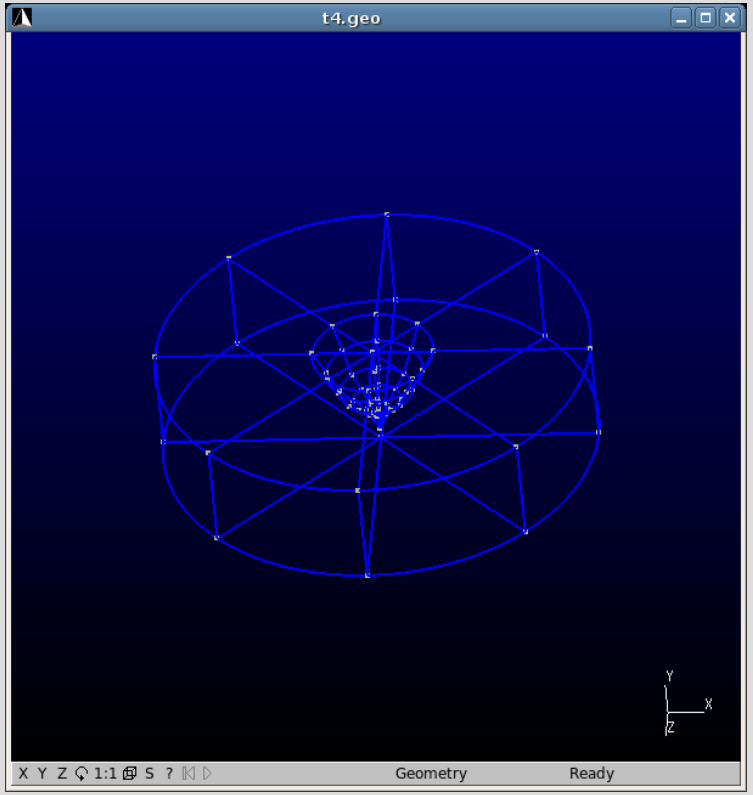
New Open Save Print... Undo Redo

t4.geo

```
Point(1) = {-0.9, 0.6, 0, 0.1};
Point(2) = {-0.9, -0.3, 0, 0.1};
Point(3) = {0.9, -0.3, 0, 0.1};
Point(4) = {0.9, 0.6, 0, 0.1};
Point(5) = {-0.4, 0.6, 0, 0.1};
Point(6) = {-0.5, 0.4, 0, 0.1};
Point(7) = {-0.6, 0.2, 0, 0.1};
Point(8) = {-0.7, 0.1, 0, 0.1};
Point(9) = {-0.8, 0, 0, 0.1};
Point(10) = {-0.9, -0.2, 0, 0.1};
Line(1) = {2,3};
Line(2) = {3,4};
Line(3) = {4,5};
Line(4) = {5,1};
Line(5) = {1,10};
Line(6) = {10,2};
Line(7) = {10,9};
Line(8) = {9,8};
Line(9) = {8,7};
Line(10) = {7,6};
Line(11) = {6,5};
Line Loop(12) = {3,-11,-10,-9,-8,-7,6,1,2};
Plane Surface(13) = {12};
Line Loop(14) = {4,5,7,8,9,10,11};
Plane Surface(15) = {14};
Extrude {{0,1,0}, {-0.9,0,0}, Pi/4} {
  Surface{13,15};
}
Extrude {{0,1,0}, {-0.9,0,0}, Pi/4} {
  Surface{57,89};
}
Extrude {{0,1,0}, {-0.9,0,0}, Pi/4} {
  Surface{131,163};
}
Extrude {{0,1,0}, {-0.9,0,0}, Pi/4} {
  Surface{237,205};
}
Extrude {{0,1,0}, {-0.9,0,0}, Pi/4} {
  Surface{311,269};
}
Extrude {{0,1,0}, {-0.9,0,0}, Pi/4} {
  Surface{385,353};
}
Extrude {{0,1,0}, {-0.9,0,0}, Pi/4} {
  Surface{417,459};
}
Extrude {{0,1,0}, {-0.9,0,0}, Pi/4} {
  Surface{491,533};
}
Surface Loop(606) = {177,103,29,578,505,431,325,283,-268,181,107,33,
-564,-490,-416,329,333,-264,185,111,37,-560,-486,-412,-408,337,-260,
189,115,41,-556,-482,-478,-404,341,-256,193,119,45,-552,-548,-474,-4
00,344,-252,196,122,48,310,204,130,56,605,532,458,352,348,306,200,12
6,52,601,528,454};
Volume(607) = {606};
Surface Loop(608) = {329,-268,181,107,33,-564,-490,-416,-396,-470,-5
44,-68,-142,-216,-248,-364,-412,333,-264,185,111,37,-560,-486,-482,-
408,337,-260,189,115,41,-556,-552,-478,-404,341,-256,193,119,45,48,1
22,196,-252,344,-400,-474,-548};
Volume(609) = {608};
```

Ln 54, Col 1 INS

gmsh



Gmsh to Femlab

t4.geo (~/femlab/grain1) - gedit

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t4.geo

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  Surface{57,89};
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}
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  Surface{385,353};
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Extrude {{0,1,0}, {-0.9,0,0}, Pi/4} {
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Extrude {{0,1,0}, {-0.9,0,0}, Pi/4} {
  Surface{491,533};
}
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-564,-490,-416,329,333,-264,185,111,37,-560,-486,-412,-408,337,-260,
189,115,41,-556,-482,-478,-404,341,-256,193,119,45,-552,-548,-474,-4
00,344,-252,196,122,48,310,204,130,56,605,532,458,352,348,306,200,12
6,52,601,528,454};
Volume(607) = {606};
Surface Loop(608) = {329,-268,181,107,33,-564,-490,-416,-396,-470,-5
44,-68,-142,-216,-248,-364,-412,333,-264,185,111,37,-560,-486,-482,-
408,337,-260,189,115,41,-556,-552,-478,-404,341,-256,193,119,45,48,1
22,196,-252,344,-400,-474,-548};
Volume(609) = {608};
```

Ln 54, Col 1 INS

python script

t.m (~/femlab/grain1) - gedit

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t4.geo t.m

```
flclear fem

% COMSOL version
clear vrsn
vrsn.name = 'COMSOL 3.2';
vrsn.ext = '';
vrsn.major = 0;
vrsn.build = 222;
vrsn.rcs = '$Name:  $';
vrsn.date = '$Date: 2005/09/01 18:02:30 $';
fem.version = vrsn;

f13P0f1=curve2([0,1.8],[0,0]);
f13P0f2=curve2([1.8,1.23350113847e-16],[0,0.1]);
f13P0f3=curve2([1.23350113847e-16,0],[0.1,0]);
f13P0g4=geomcoerce('solid',{f13P0f1,f13P0f2,f13P0f3});
f13P0=embed(f13P0g4,'Wrkpln',[-0.9 0.9 -0.9; -0.3 -0.3 -0.2; 0.
0 0.0 0.0]);
f13P1f1=curve2([0,1.80277563773],[0,0]);
f13P1f2=curve2([1.80277563773,0.00554700196225],[0,0.09984603532
05]);
f13P1f3=curve2([0.00554700196225,0],[0.0998460353205,0]);
f13P1g4=geomcoerce('solid',{f13P1f1,f13P1f2,f13P1f3});
f13P1=embed(f13P1g4,'Wrkpln',[0.9 -0.9 0.9; -0.3 -0.2 -0.2; 0.0
0.0 0.0]);
f13P2f1=curve2([0,1.8],[0,0]);
f13P2f2=curve2([1.8,0.1],[0,0.2]);
f13P2f3=curve2([0.1,0],[0.2,0]);
f13P2g4=geomcoerce('solid',{f13P2f1,f13P2f2,f13P2f3});
f13P2=embed(f13P2g4,'Wrkpln',[-0.9 0.9 -0.8; -0.2 -0.2 0.0; 0.0
0.0 -0.0]);
f13P3f1=curve2([0,1.71172427686],[0,0]);
f13P3f2=curve2([1.71172427686,0.0233682495135],[0,0.19863012086
5]);
f13P3f3=curve2([0.0233682495135,0],[0.198630120865,0]);
f13P3g4=geomcoerce('solid',{f13P3f1,f13P3f2,f13P3f3});
f13P3=embed(f13P3g4,'Wrkpln',[0.9 -0.8 0.9; -0.2 0.0 0.0; 0.0 -
0.0 0.0]);
f13P4f1=curve2([0,1.7],[0,0]);
f13P4f2=curve2([1.7,0.1],[0,0.1]);
f13P4f3=curve2([0.1,0],[0.1,0]);
f13P4g4=geomcoerce('solid',{f13P4f1,f13P4f2,f13P4f3});
f13P4=embed(f13P4g4,'Wrkpln',[-0.8 0.9 -0.7; 0.0 0.0 0.1; -0.0
0.0 -0.0]);
f13P5f1=curve2([0,1.60312195419],[0,0]);
f13P5f2=curve2([1.60312195419,0.0062378028615 52],[0,0.09980525784
83]);
f13P5f3=curve2([0.0062378028615 52,0],[0.0998052578483,0]);
f13P5g4=geomcoerce('solid',{f13P5f1,f13P5f2,f13P5f3});
f13P5=embed(f13P5g4,'Wrkpln',[0.9 -0.7 0.9; 0.0 0.1 0.1; 0.0 -0.
0 0.0]);
f13P6f1=curve2([0,1.6],[0,0]);
f13P6f2=curve2([1.6,0.1],[0,0.1]);
f13P6f3=curve2([0.1,0],[0.1,0]);
f13P6g4=geomcoerce('solid',{f13P6f1,f13P6f2,f13P6f3});
f13P6=embed(f13P6g4,'Wrkpln',[-0.7 0.9 -0.6; 0.1 0.1 0.2; -0.0
0.0 -0.0]);
f13P7f1=curve2([0,1.50332963784],[0,0]);
f13P7f2=curve2([1.50332963784,0.0066519010523 8],[0,0.09977851578
57]);
f13P7f3=curve2([0.0066519010523 8,0],[0.0997785157857,0]);
f13P7g4=geomcoerce('solid',{f13P7f1,f13P7f2,f13P7f3});
```

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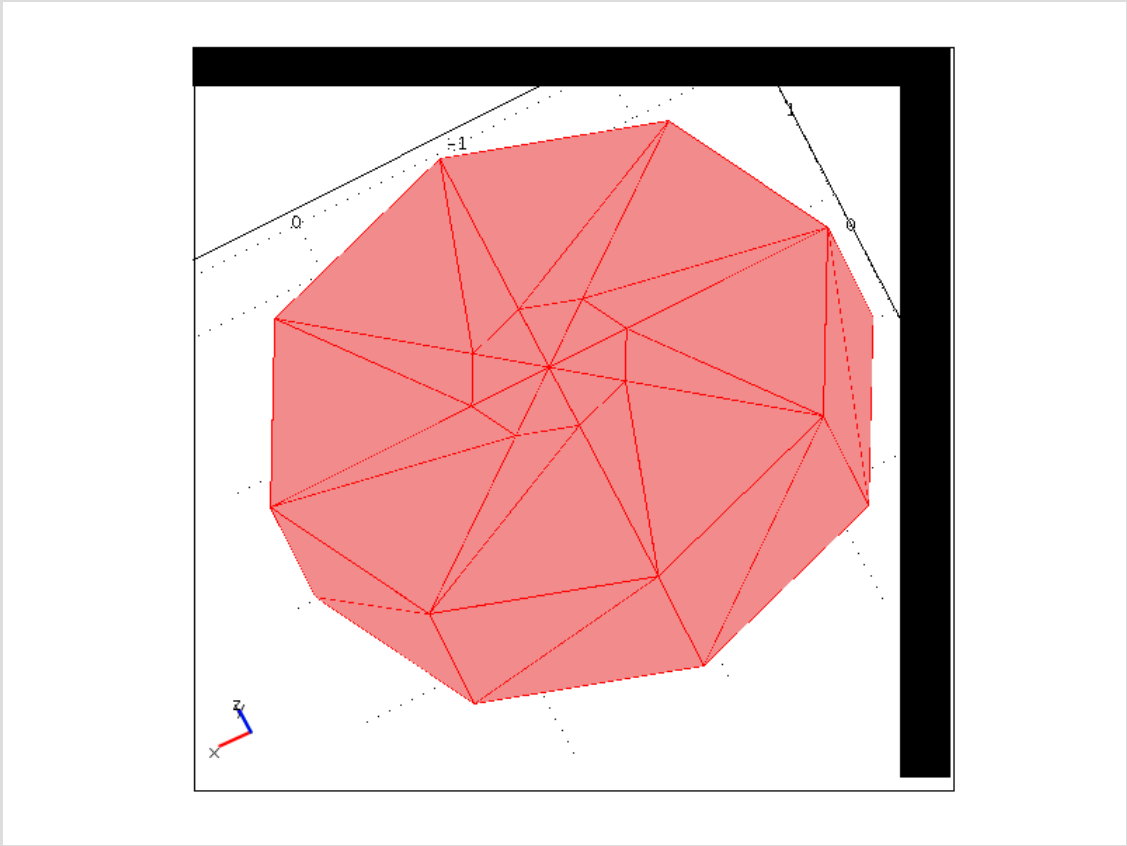
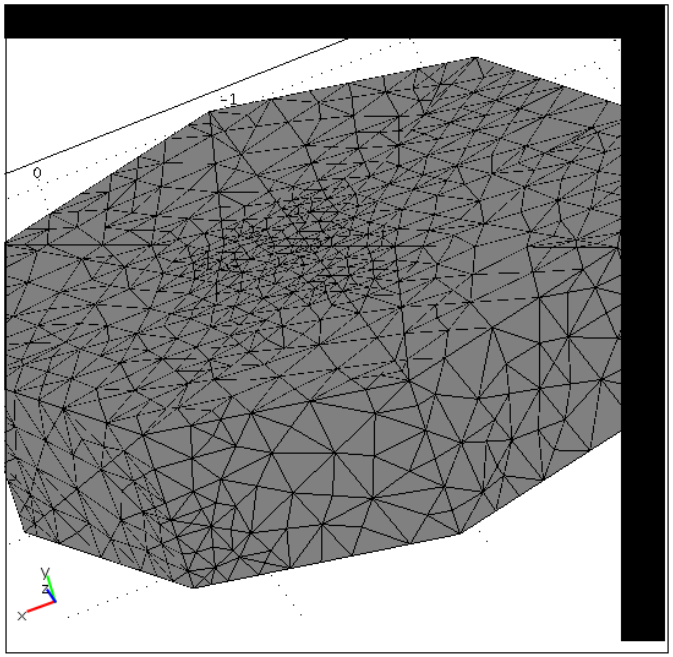
+40 times more screens....

Load into Femlab



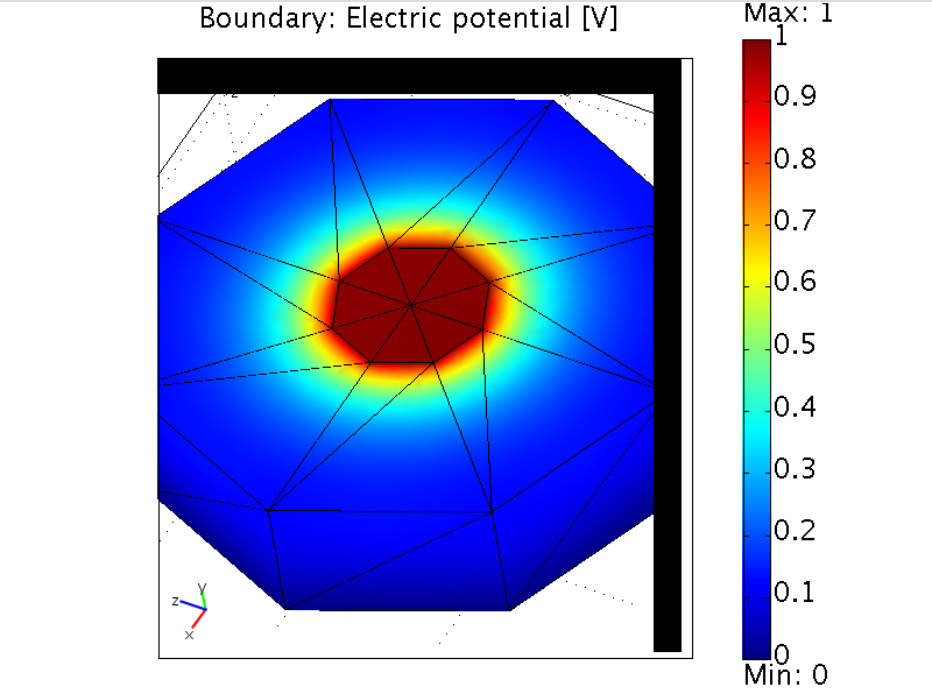
takes 60s to load compared to less than 1s in gmsh...

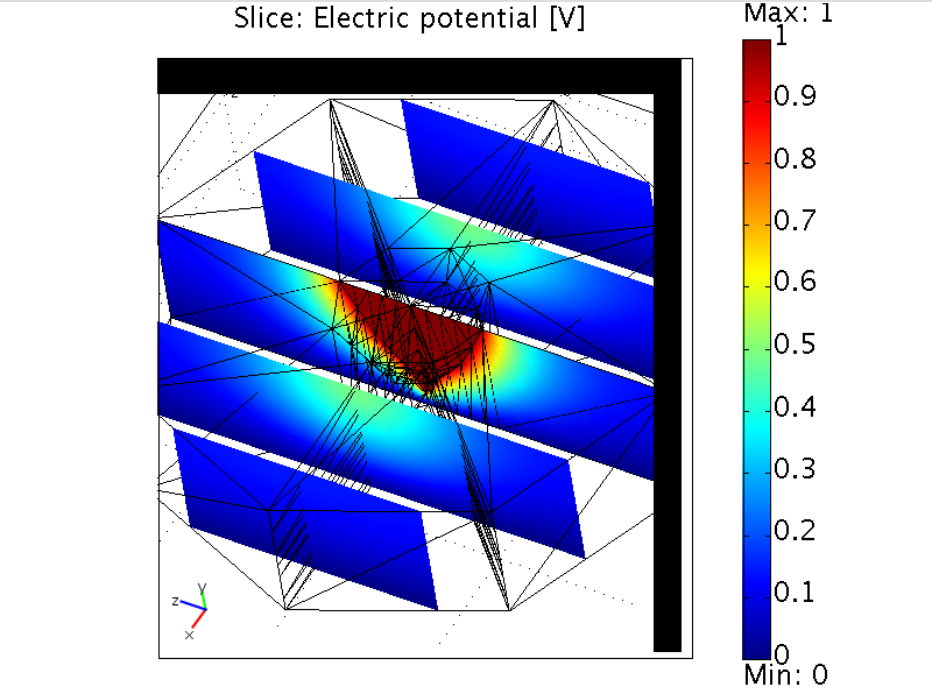
Mesh



Solution

we apply a voltage at the high conductive grain





Conclusion

- femlab scripting abilities very poor:
  - sometimes it falls down
  - error messages unmeaningful, line numbers missing
  - bug in face3 renders femlab almost unusable
- nevertheless, FEM features are really useful and work well