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# Modeling of Random Nanostructures Based on SEM Images and Analysis of Resulting RF Performance

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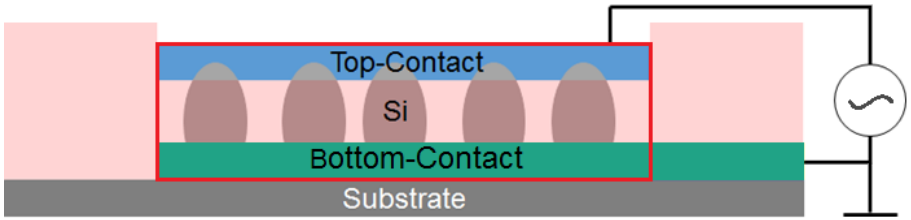
COMSOL CONFERENCE 2018 LAUSANNE

DFG Deutsche Forschungsgemeinschaft
German Research Foundation

# Introduction

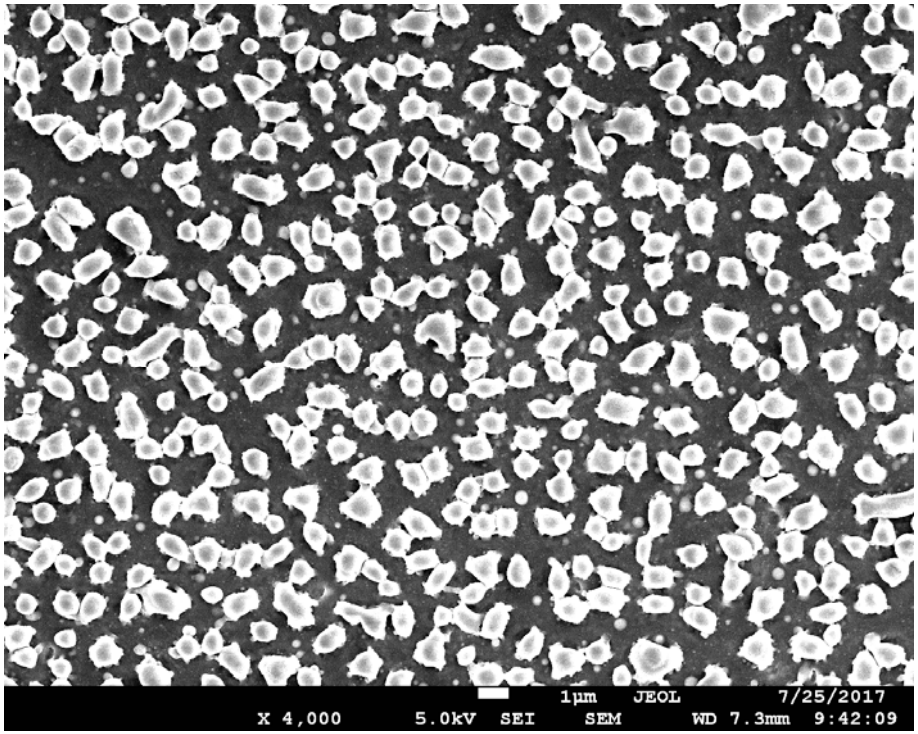
- Goal: Printable radio frequency rectifier
- Silicon nanoparticles → laser sintered → cone like structures
- Potential Schottky diodes




- Geometry →
  Parasitic capacitances →
  Limit cut-off frequency

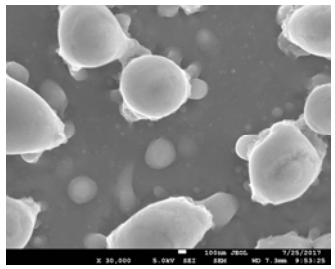
Is this approach suitable for RF applications?

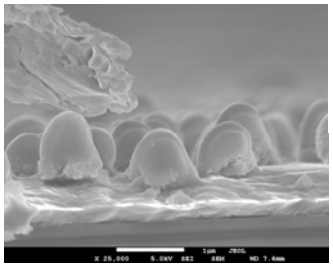
Top view SEM image of Si-cones



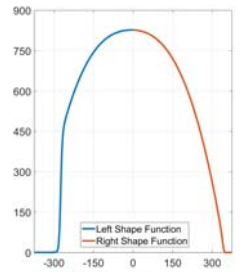
# Workflow

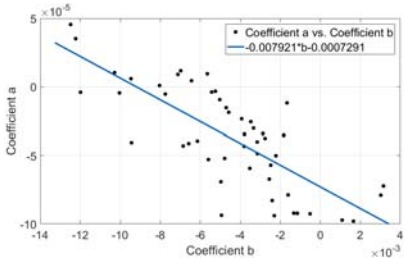
SEM Image Analysis
- Top view → footprints
- Cross cut → shape functions



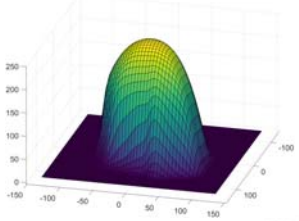


Mathematical representation
Stochastic formulation

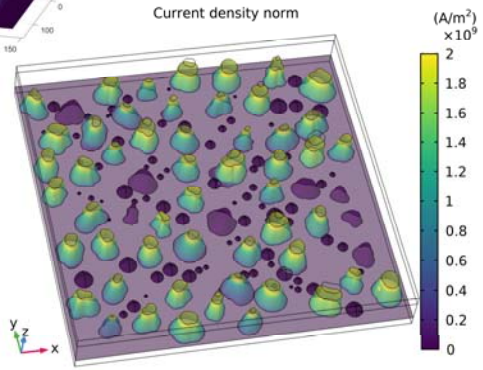


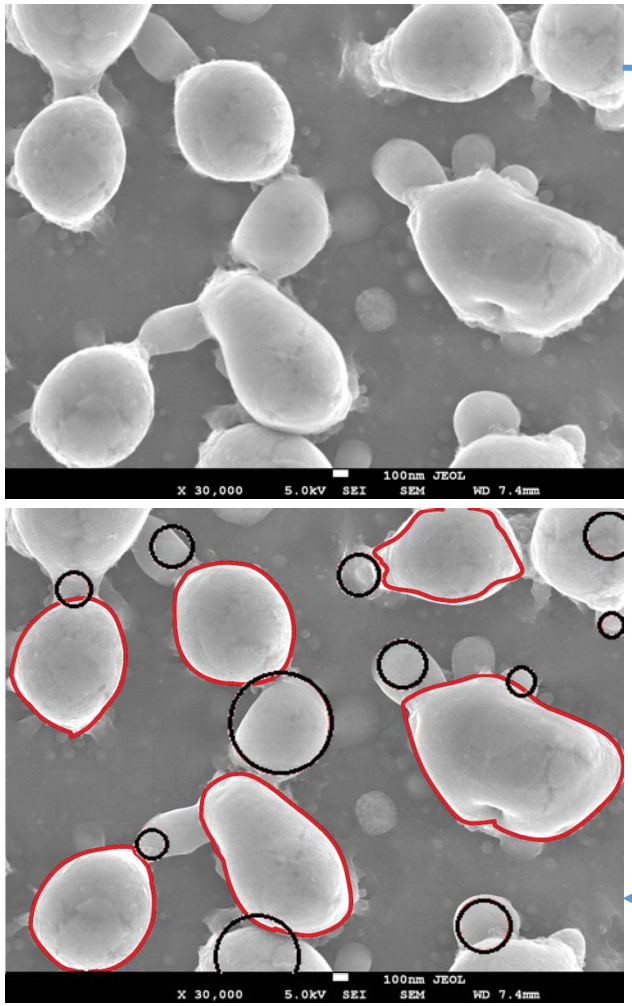

Random 3D surface generation in MATLAB®



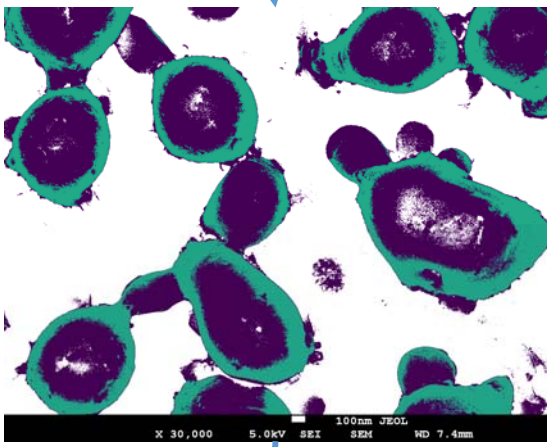
LiveLink™ *for* MATLAB®
- One cone model
- Multi cone model



# Image Analysis – Top View



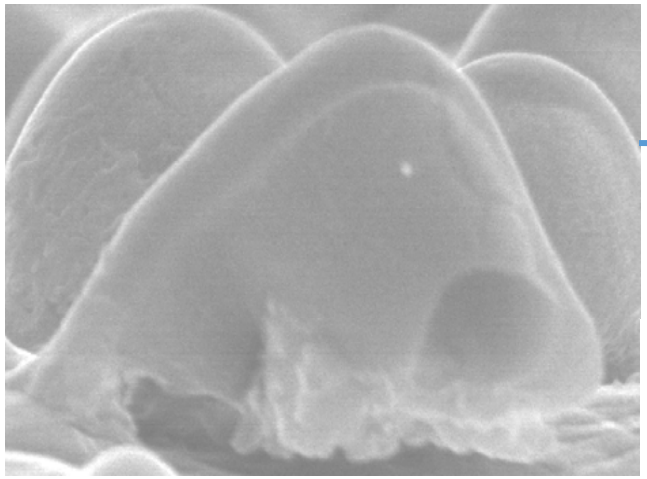

Multilevel thresholding




Edge detection and Morphological opening/closing operations

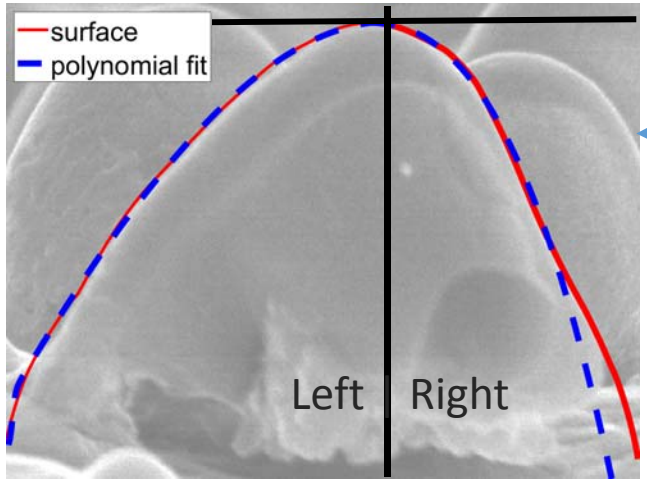
1. Footprint = function of angle and distance from center (polar coordinates)
2. Extraction of droplets (tiny structures that do not form cones)

# Image Analysis – Cross Cut



Thresholding +
Edge detection

Morphological
operations +
edge detection




$$y(x) = (a \cdot x^3 + b \cdot x^2 + c \cdot x + d) \cdot \frac{1}{1 + e^{x+w}}$$

Coefficient *d* = height of the cone

→ 4 coefficients to fit (*a*,*b*,*c*,*w*)

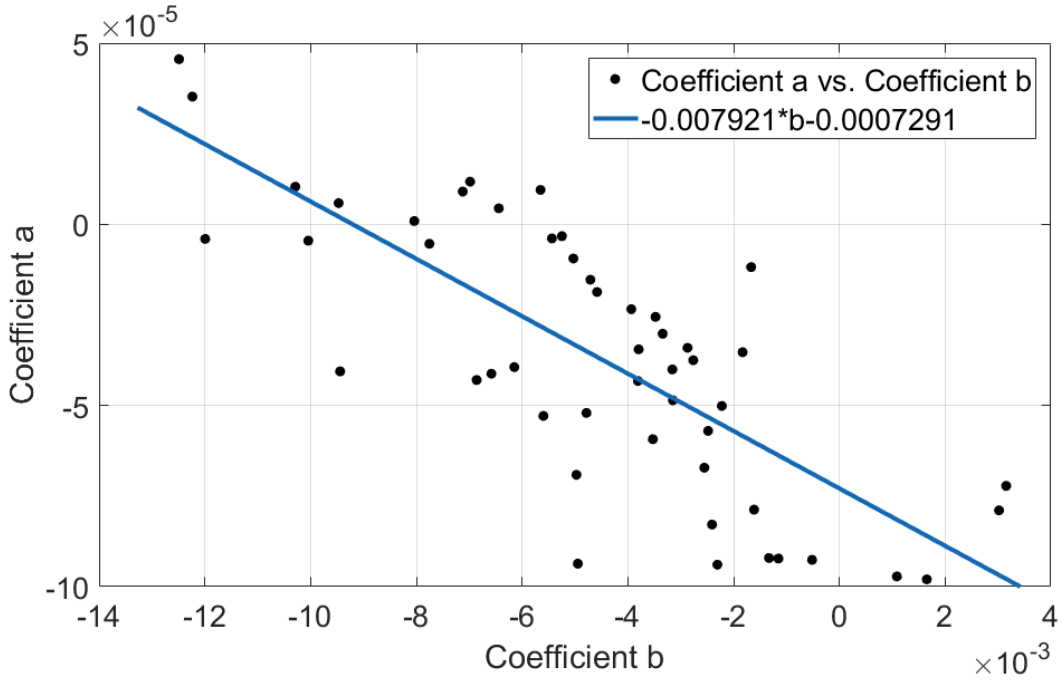
- Shape extraction of front cone
- Fit both halves with a combination of polynomial and sigmoid function

# Correlation

- 50 extracted shape functions with different coefficients

→ normal distributions

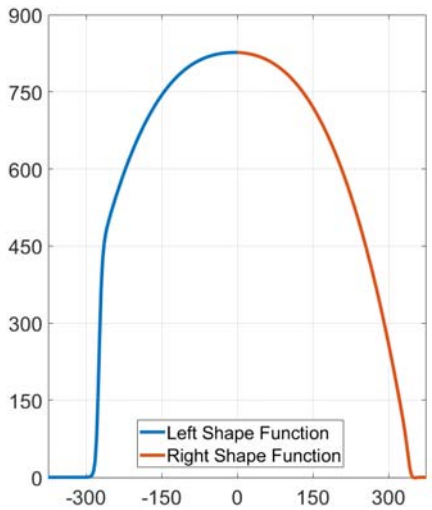
- Every structure is different but all follow a conical shape
- Correlation between coefficients?



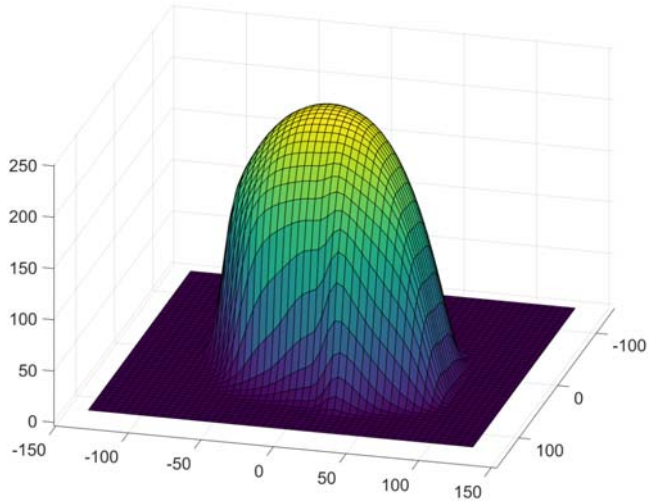

- Coefficient *b* exhibits the strongest correlation to the other coefficients

For random shape generation: correlation function *f(b)* has to be incorporated!

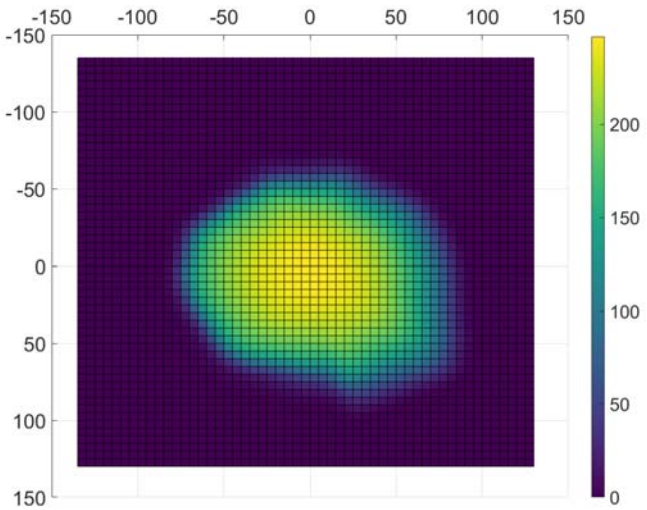
# Random 3D Model Generation




shape functions



3D view



top view

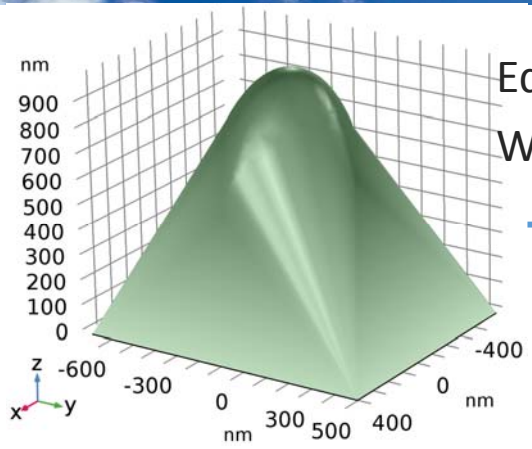
- Randomly generated shape functions
- Rotation by 180 degrees
- Use morph function *μ(α)* to avoid discontinuities
- *z*: insert *r'* – footprint function
- Export .txt file for usage in COMSOL Multiphysics®

$$\mu(\alpha) = \frac{1}{1 + 3 \cdot e^{\alpha + \frac{\pi}{2}}}$$

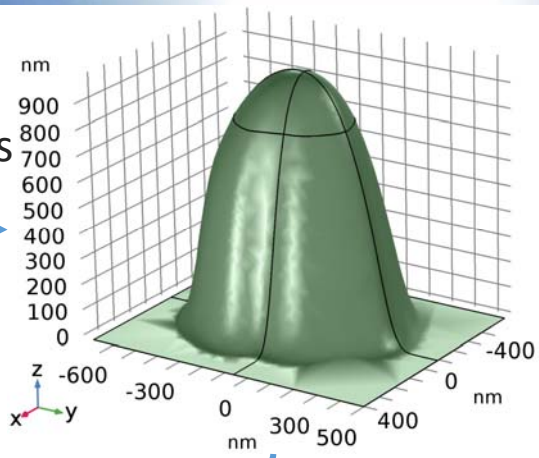
$$z(r', \alpha) = \mu(\alpha) \cdot y_{left}(r') + \ldots (1 - \mu(\alpha)) \cdot y_{right}(r')$$

# One Cone Model

- Import as interpolation from file
- Parametric surface using this function

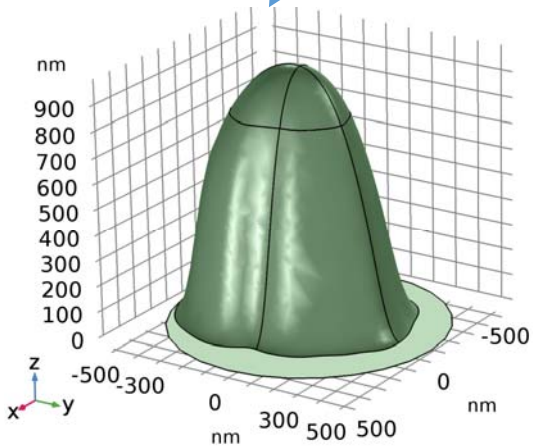



Edge partition
Workplane cuts

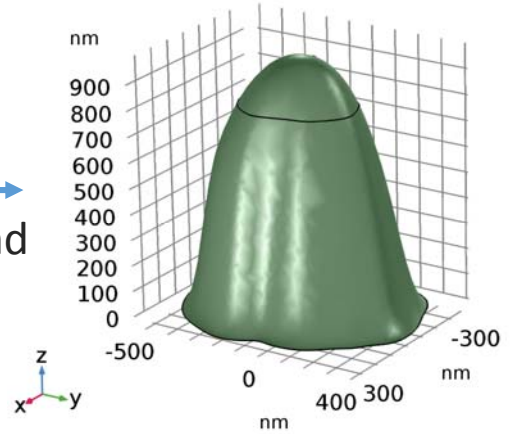



Convert to solid
(with a cylinder)

Top workplane cut
→ seperate dielectric and top metal contact




selections and deletions




Save individual cone as .mphbin file

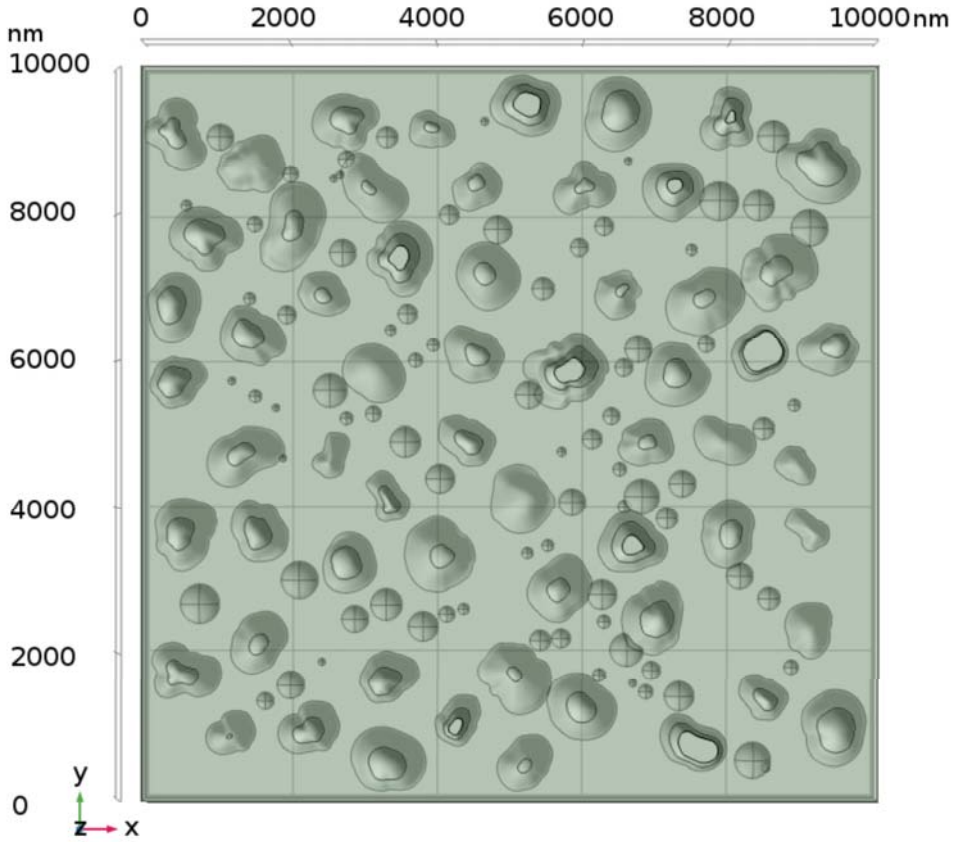
# Multi Cone Model

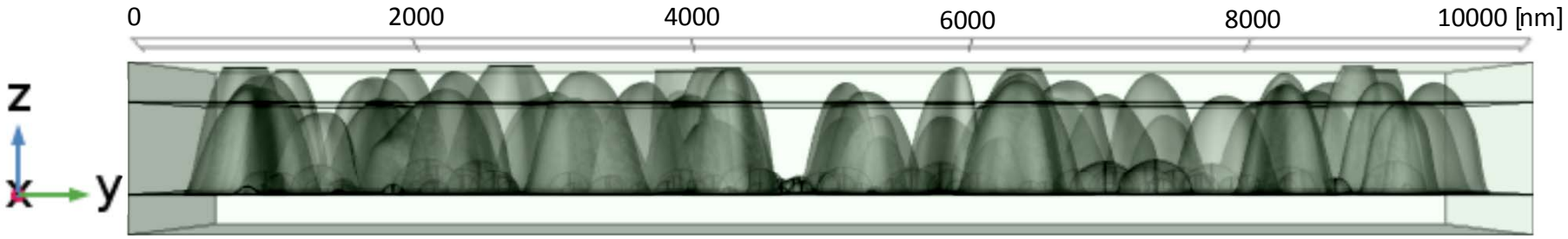
Purpose:

- Viable for RF-rectifier?
- Only parasitic capacitances

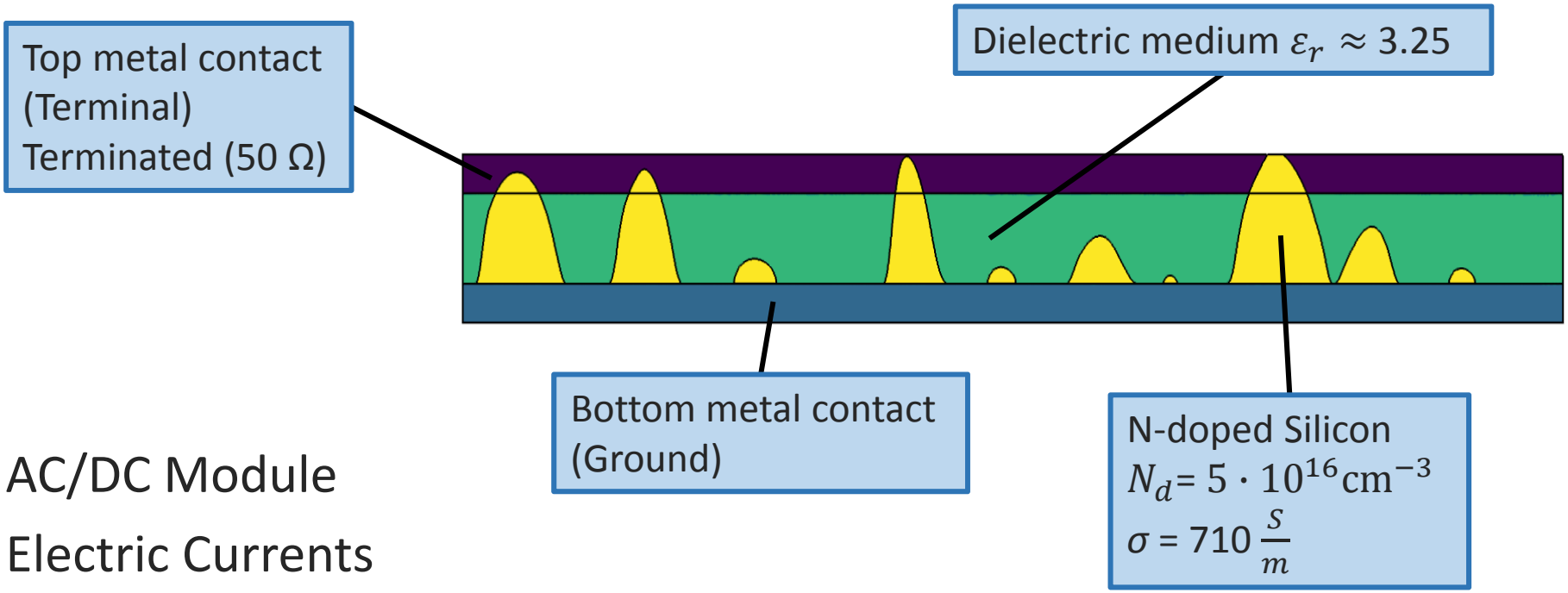
LiveLink™ *for* MATLAB®:

- Import of cone models
- Random distribution
  - across the simulation area
  - according to cone density
  - from SEM images



# Simulation Setup




- AC/DC Module
- Electric Currents
- Scattering parameters → *Y* parameters
- Frequency sweep to estimate cut-off frequency $f_c$:

  Frequency where the displacement currents predominate.

  Im {*Y*} = Re {*Y*}
- Vary geometric parameters to maximize $f_c$

# Simulation Results

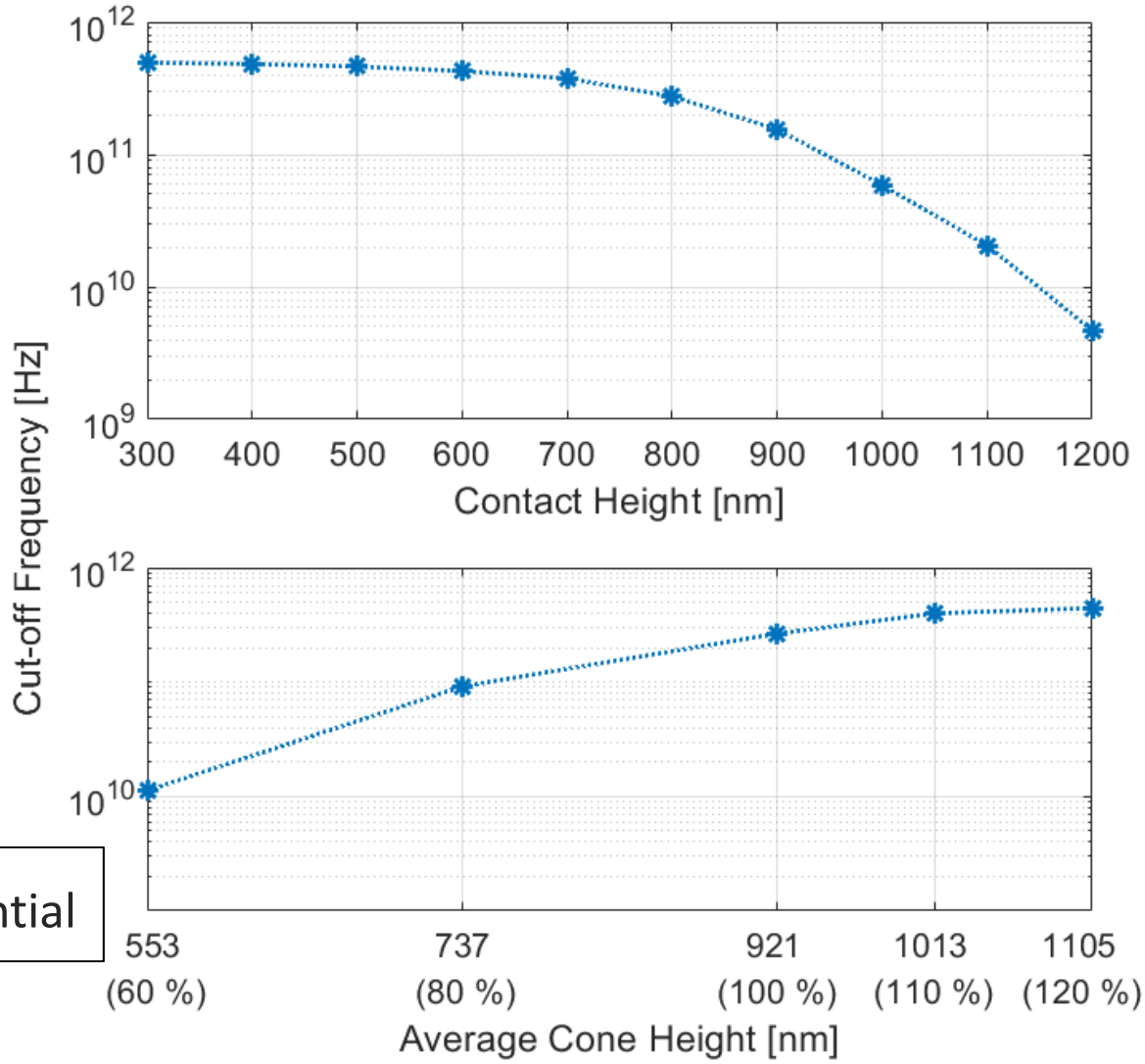
- Contact height $H_{contact}$ = distance between top and bottom contact

$$H_{contact} \downarrow \Rightarrow f_c \uparrow$$

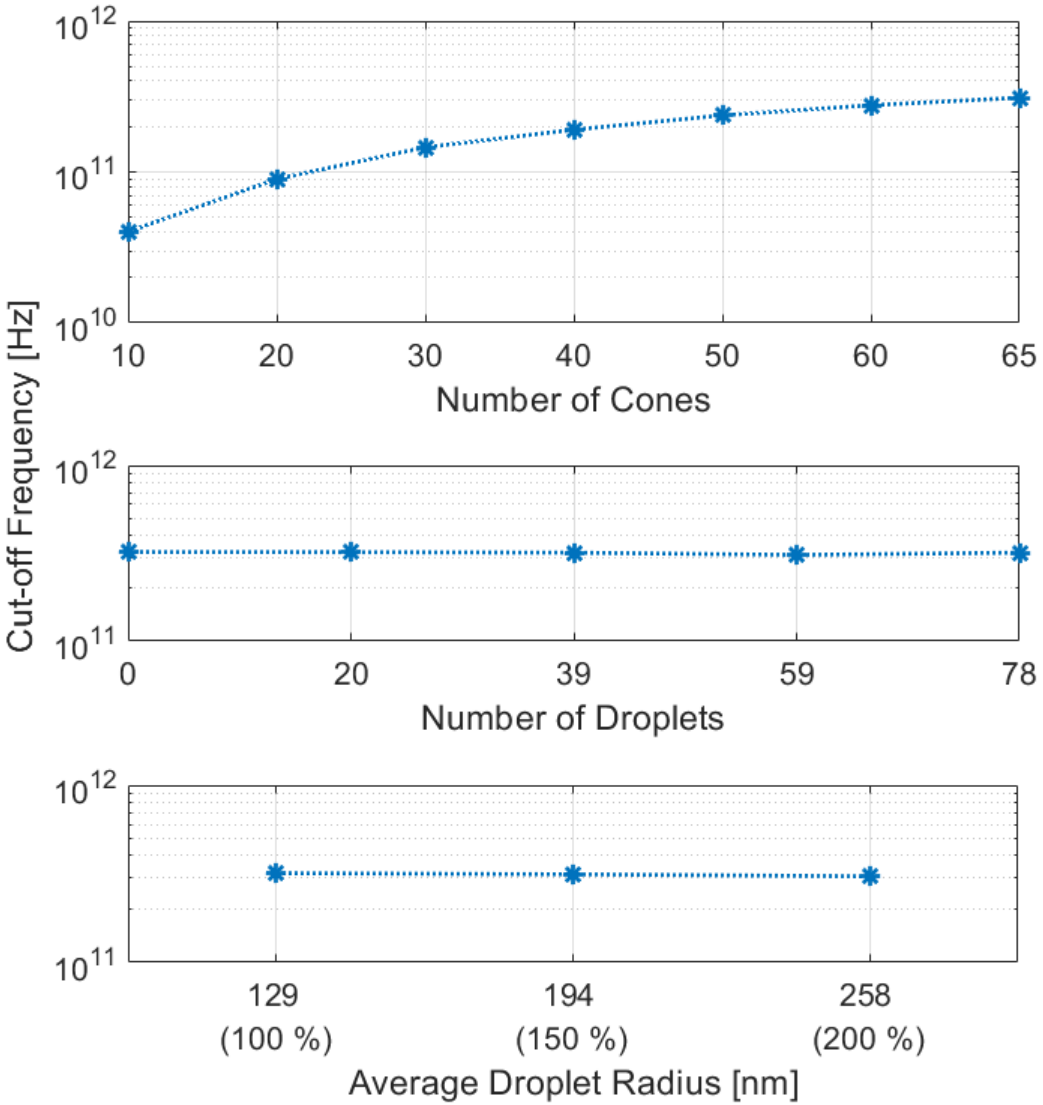
- Average cone height $\overline{H_{cone}}$

$$\overline{H_{cone}} \uparrow \Rightarrow f_c \uparrow$$

High (parasitic) $f_c$ shows RF potential



# Simulation Results




- Number of cones $N_c$

$$N_c \uparrow \Rightarrow f_c \uparrow$$

- Number of droplets $N_d$

$$N_d \updownarrow \Rightarrow f_c = \text{const}$$

- Radius of droplets $\overline{R_d}$

$$\overline{R_d} \updownarrow \Rightarrow f_c = \text{const}$$

# Conclusion

- Proposed idea suitable for realising a printable RF rectifier
- Extraction of geometry by SEM image processing
- Mathematical formulation
- Generation of random 3D models with same stastistic properties
- Model helps to optimize device:
  - Main focus should lie on contacting every cone
  - Effects of droplets do not need to be considered

# Finish

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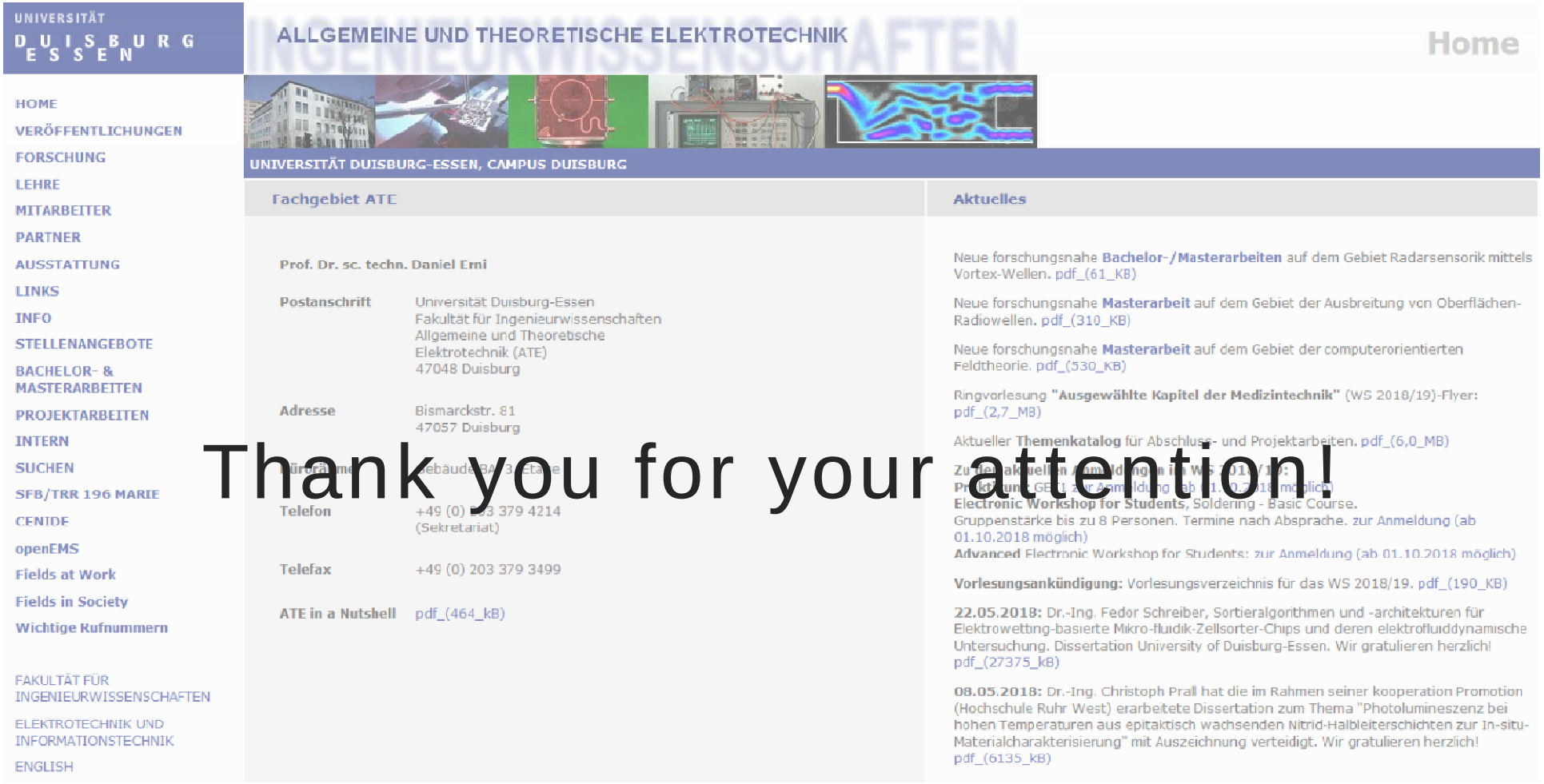


Thank you for your attention!

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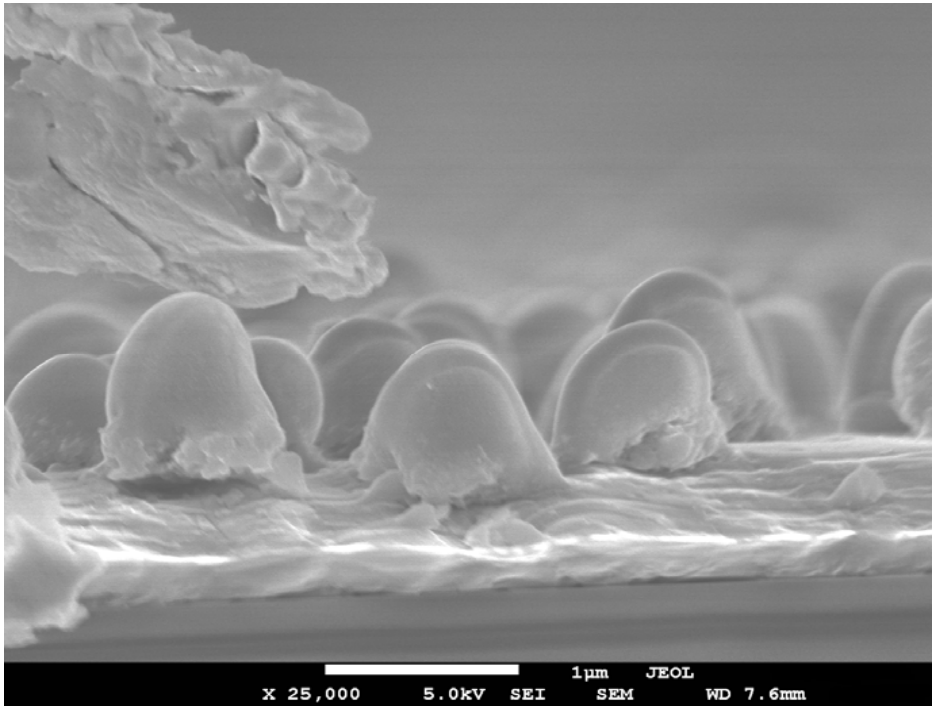
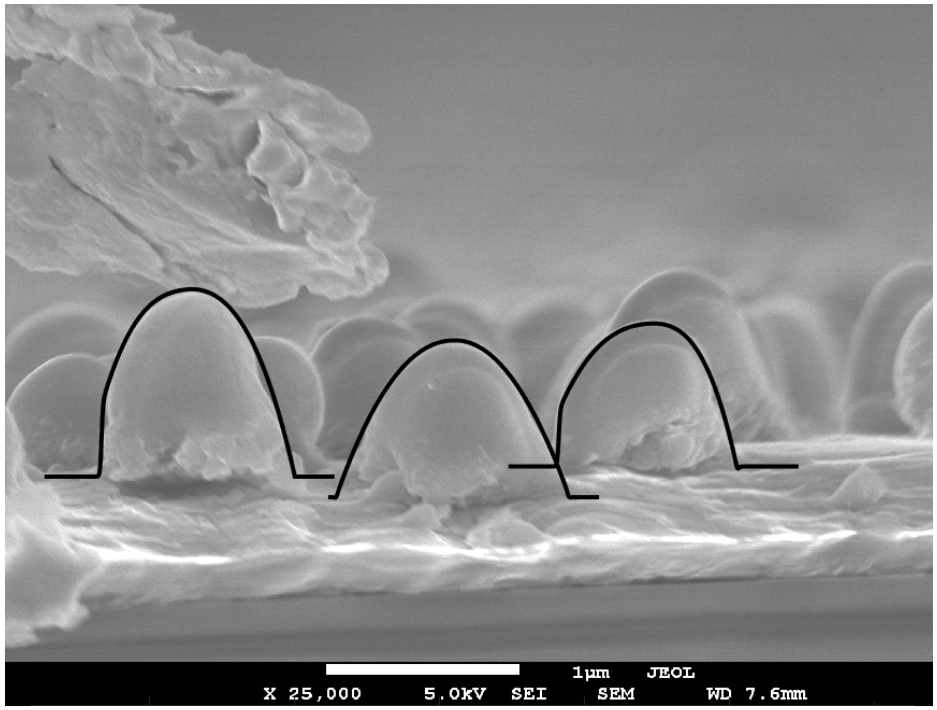
# Image Analysis – Cross Cut



# Current density

- Some cones are not in contact to the top terminal
  → can‘t carry any current

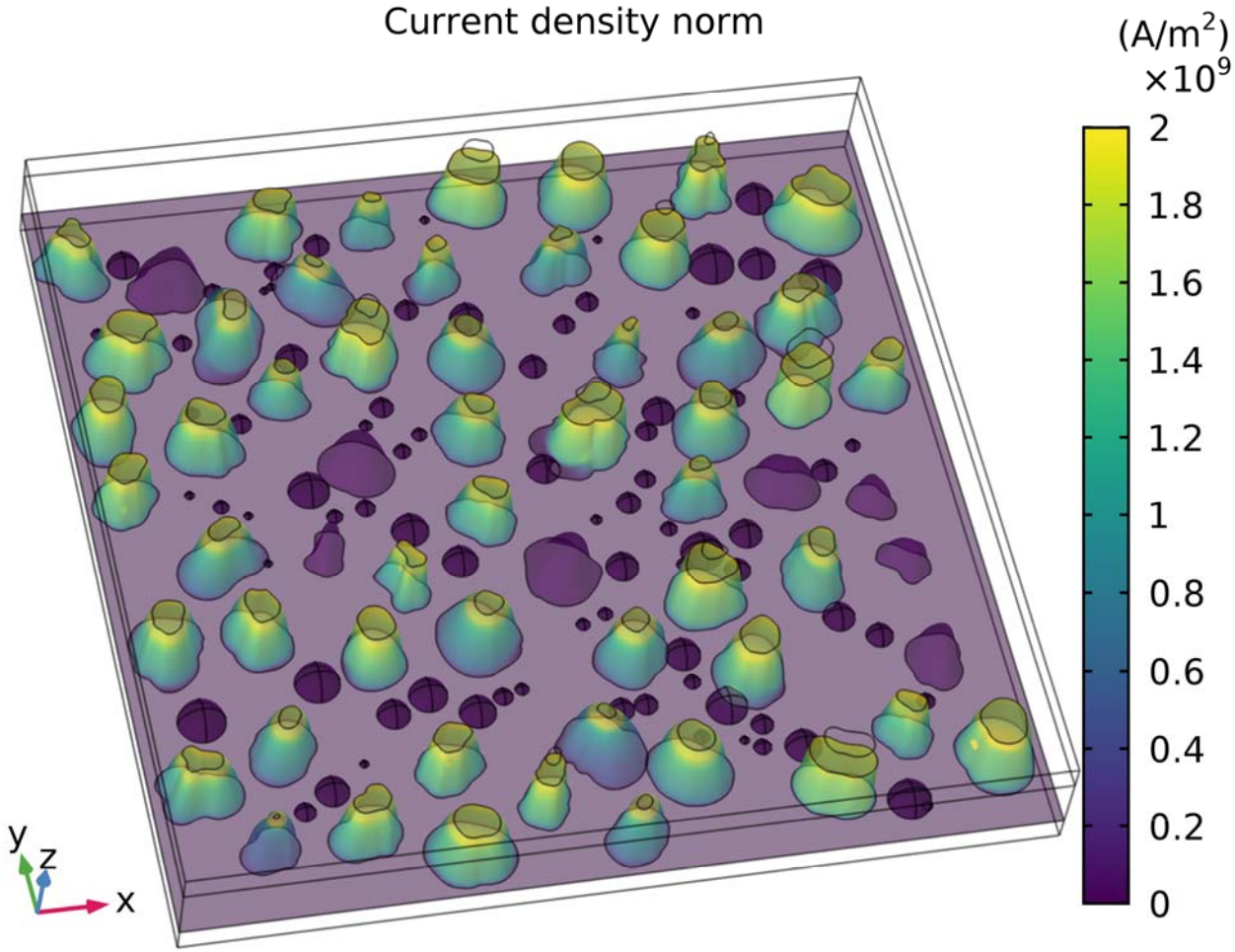



**Fig. A1**: Current desity norm @ 1 GHz between the two terminals calculated by the Electric Currents module