MNC 2015

Simulation of plastic injection for nanostructure pattern replication

Amsterdam, 9th December 2015, 14:20-14:40

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aim4np

SEVENTH FRAMEWORK PROGRAMME

Overview

1. Introduction to aim4np project
2. Simulations of plastic injection at nano level
3. Experiments of plastic injection at nano level
4. Next steps

1.- Introduction to aim4np project

Aim4np is a FP7 funded project to build an Automated In-line Metrology for (4) Nanoscale Production.

http://aim4np.eu/

1.- Introduction to aim4np project

Production enters nanometer domain

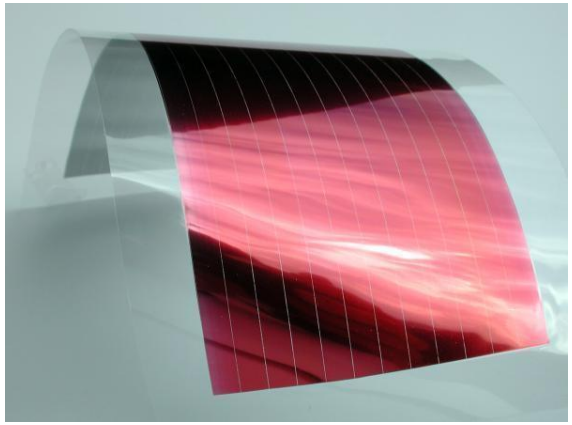


image: www.icsana.com

image: www.syntecoptics.com

Measurement of nanomechanical properties for:

- Quality control
- Tool-lifetime monitoring
- Maintaining precision
- Processing control

Crucial for an efficient production!

1.- Introduction to aim4np project

Nanomechanical properties - nmp

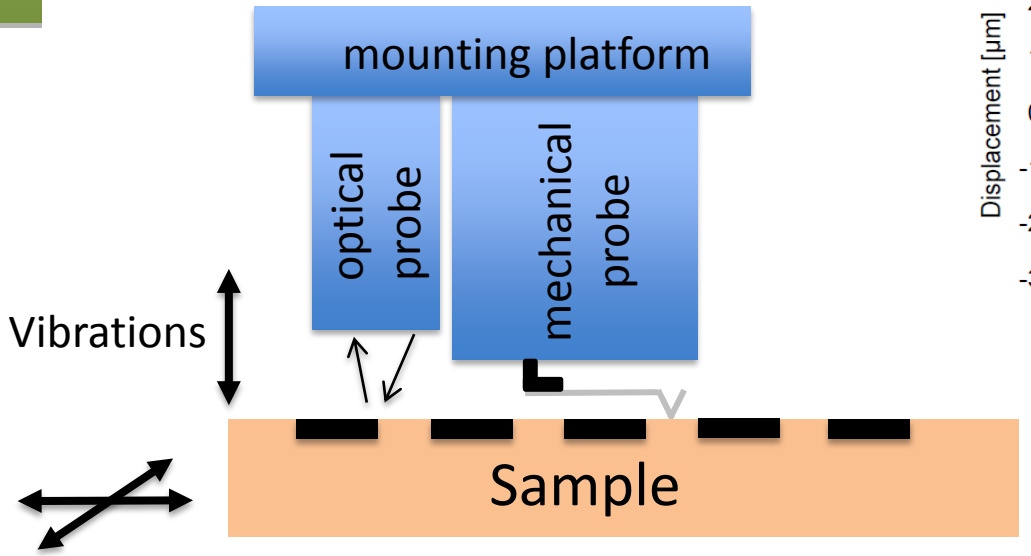
- typical or relevant length scale below 0.1µm
- macroscopic objects or nanoscale objects
- texture (roughness, ...)
- hardness, elasticity, ...

➡ Competences needed

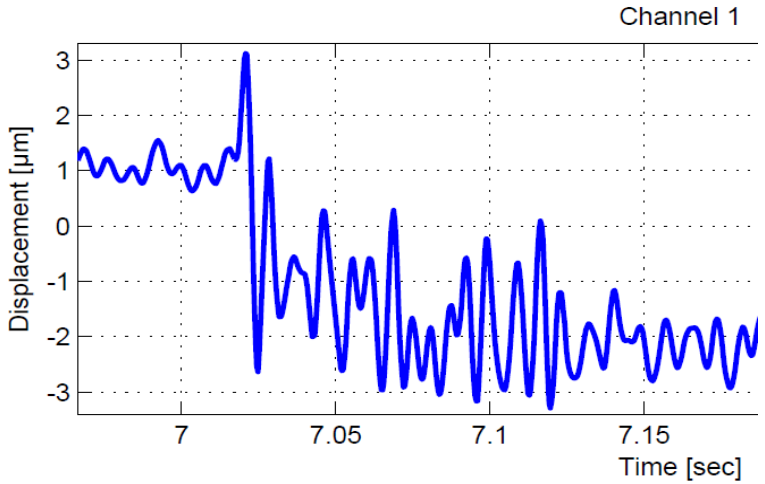
- positioning/placement on free body form
- imaging, local probing or loading
- traceability of results
- linking properties to functionality

1.- Introduction to aim4np project

Challenge



Sample vibration



Possible implementation of probes:

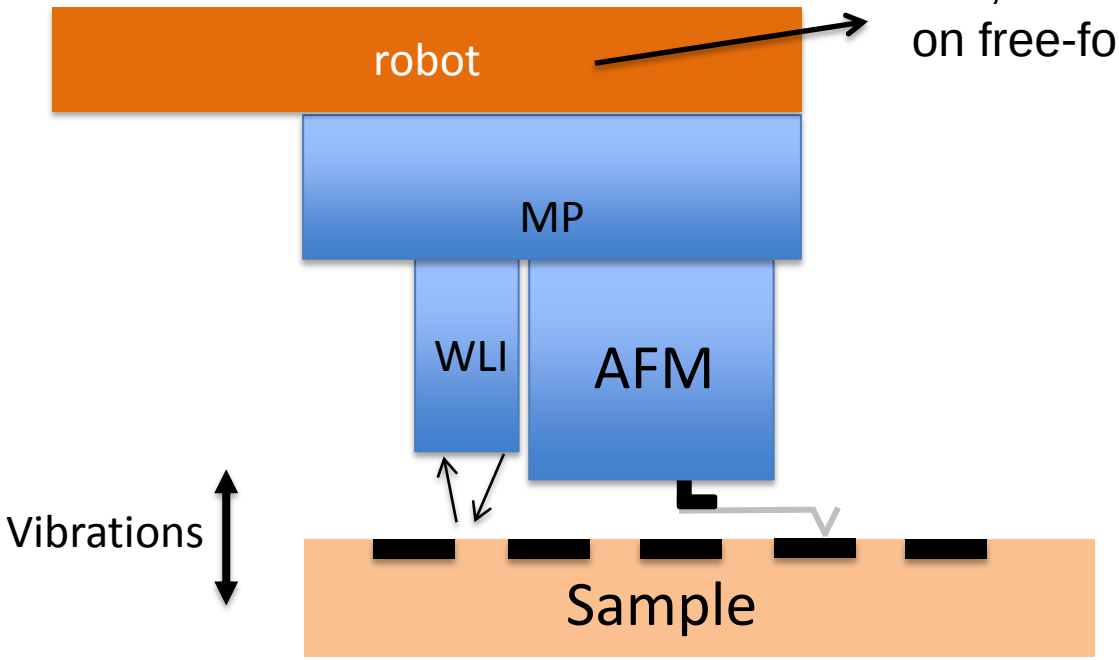
Atomic Force Microscope [AFM]

White Light Interferometer [WLI]

Environmental vibrations hinder the stable proximity needed for conducting nanomechanical measurements!

1.- Introduction to aim4np project

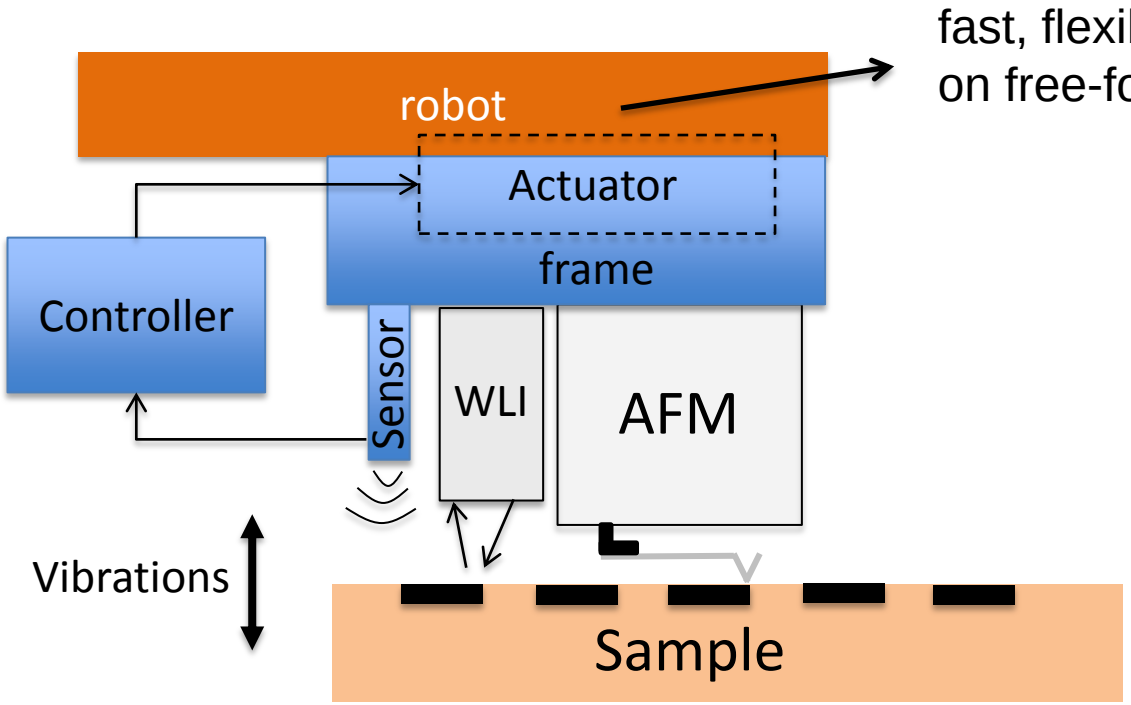
Proposed solution



AFM…Atomic Force Microscope
WLI…White Light Interferometer
MP … Metrology Platform

1.- Introduction to aim4np project

Proposed solution



- ‘artificial stiffness‘
- Tracking of sample motion within < 1µm (= 5% of AFM actuation range)

AFM…Atomic Force Microscope
WLI…White Light Interferometer
MP … Metrology Platform

1.- Introduction to aim4np project

Plastic injection application of aim4np

Plastic injection is selected as a possible application for aim4np to control moulds and plastic parts in-line to assure surface quality.

Simulations are required to decide where to do AFM measurements on mould and plastic part.

Flubetech provides DLC coatings ranging Sq=6 to 35nm.

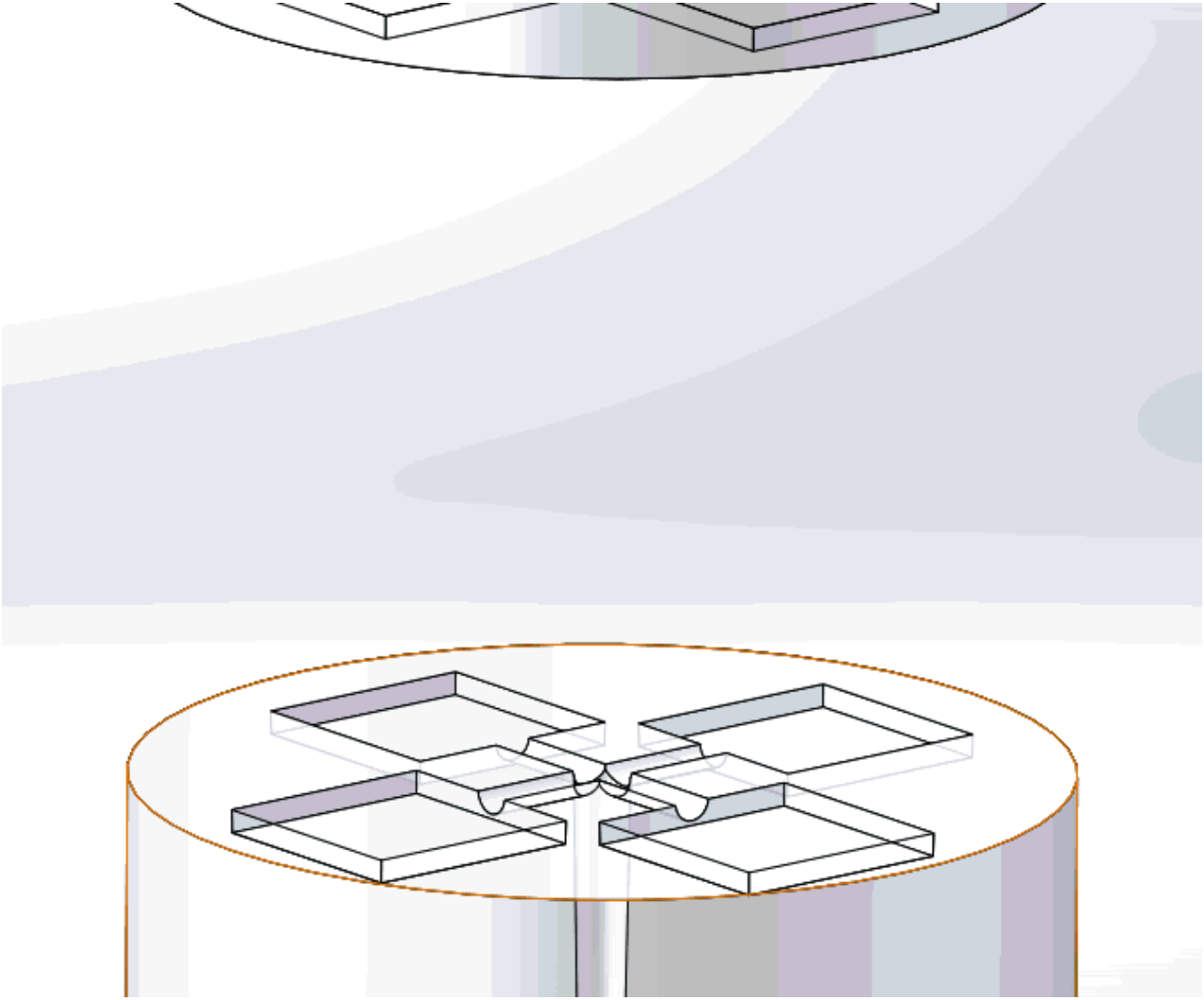
CSIC-CNM measure coating on mould Sq=6nm, and plastic parts from 4nm to 0.6nm.

IQS carries out simulations of plastic injection.

External partner plastic injection.

1.- Introduction to aim4np project

Plastic injection application of aim4np



2.- Simulations of plastic injection at nano level

Contents of Simulation:

2.1. Model to validate

2.2. Problem to do fine mesh.

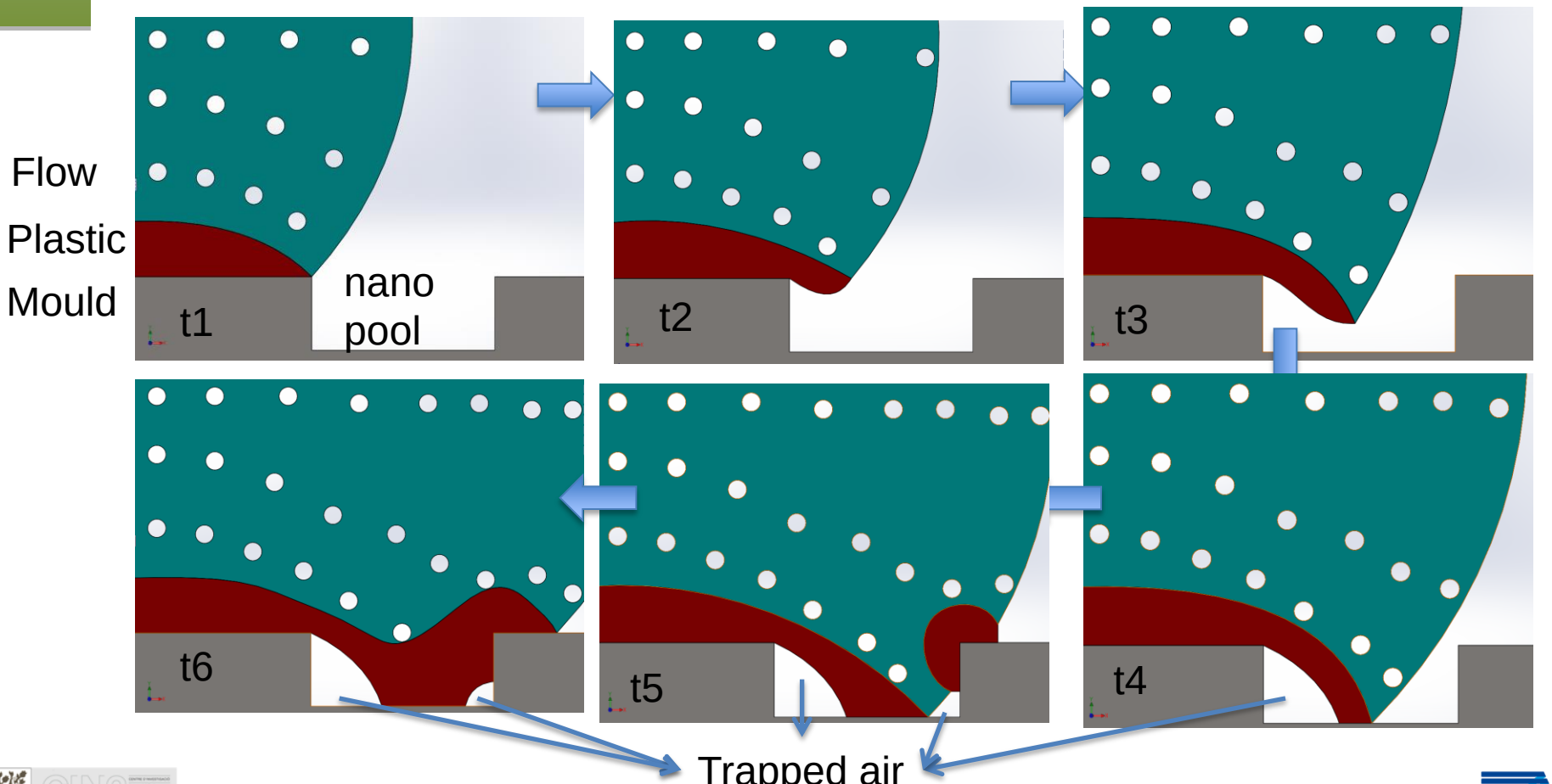
2.3. Submodelling approach.

2.4. Initial results.

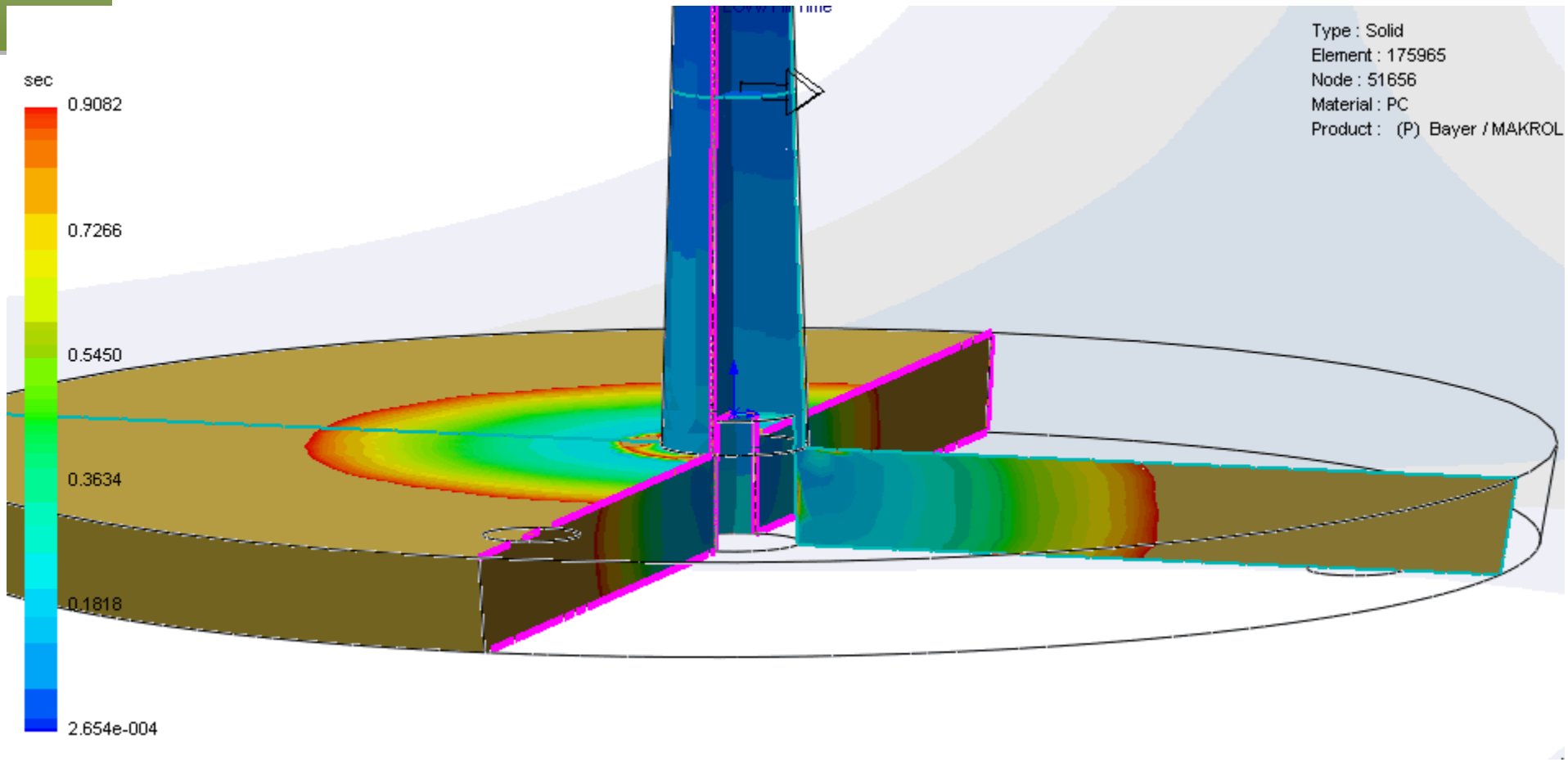
2.- Simulations of plastic injection at nano level

2.1 Model to validate

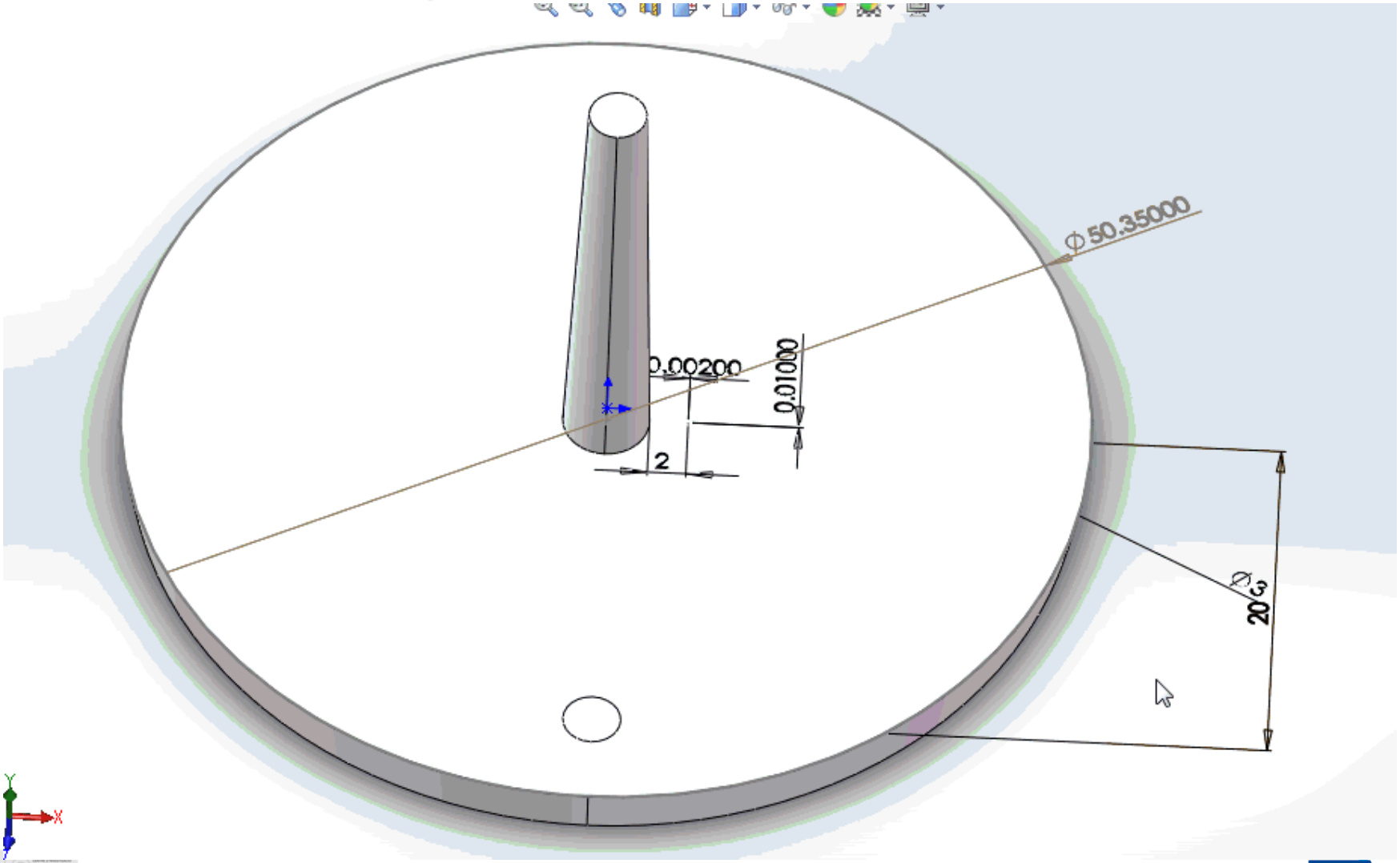
Velocity and FIB mark height are important to copy mark on plastic.



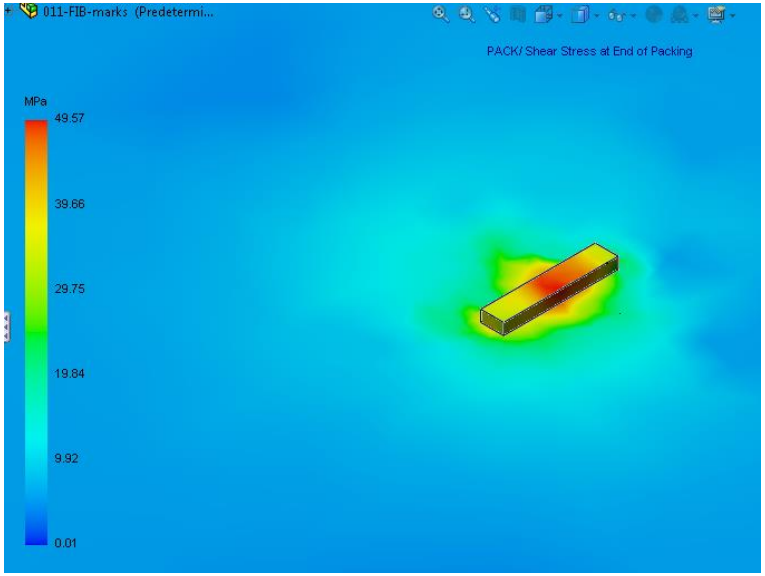
2.- Simulations of plastic injection at nano level
2.2 Fine mesh problematic

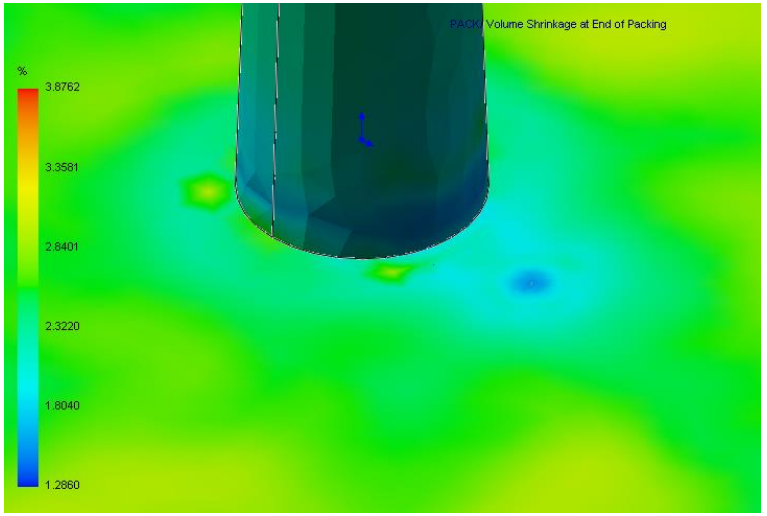


2.- Simulations of plastic injection at nano level
2.2 Fine mesh problematic



2.- Simulations of plastic injection at nano level
2.2 Fine mesh problematic

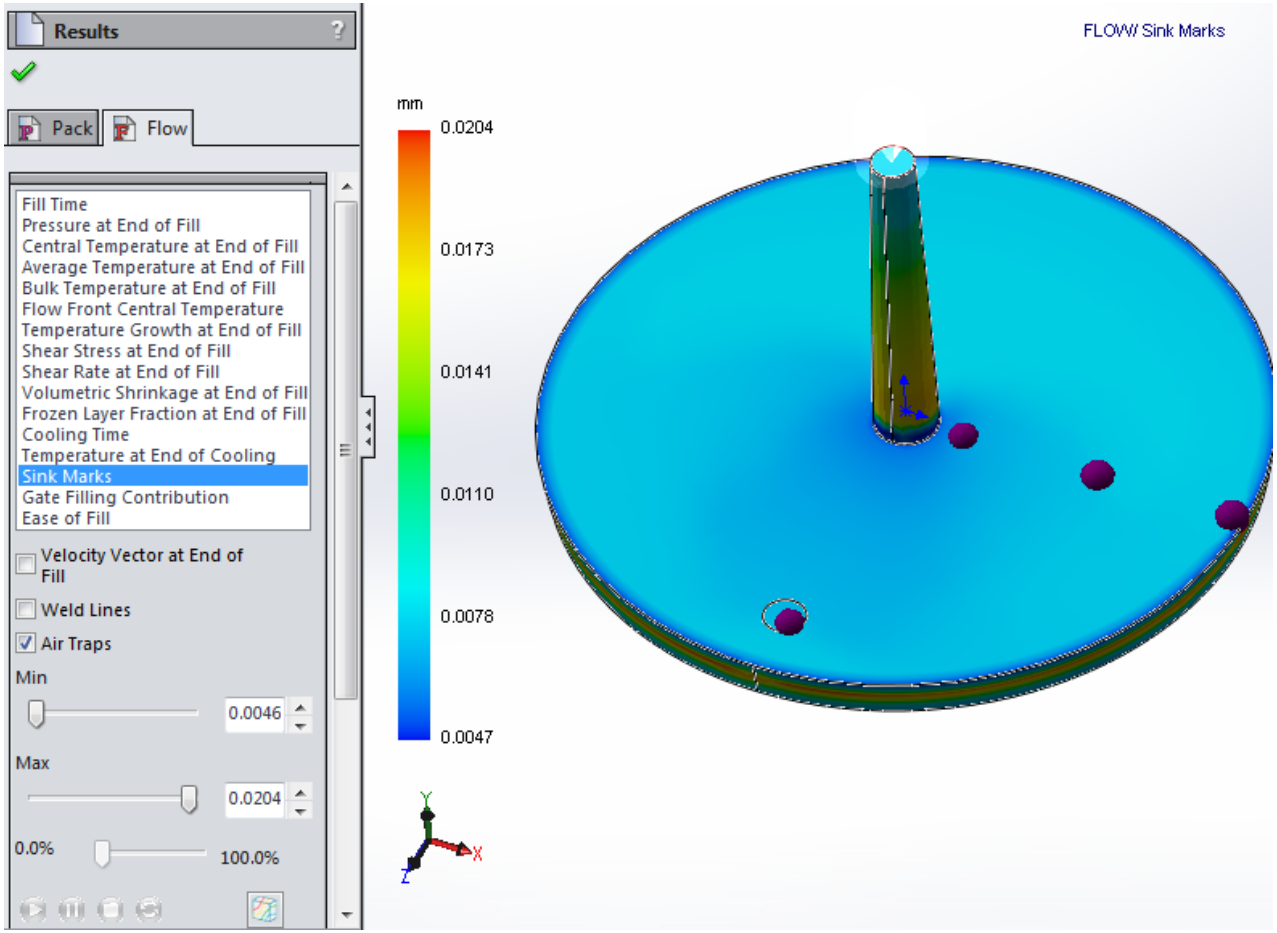




Shear stress and Volume shrinkage around control nano pool

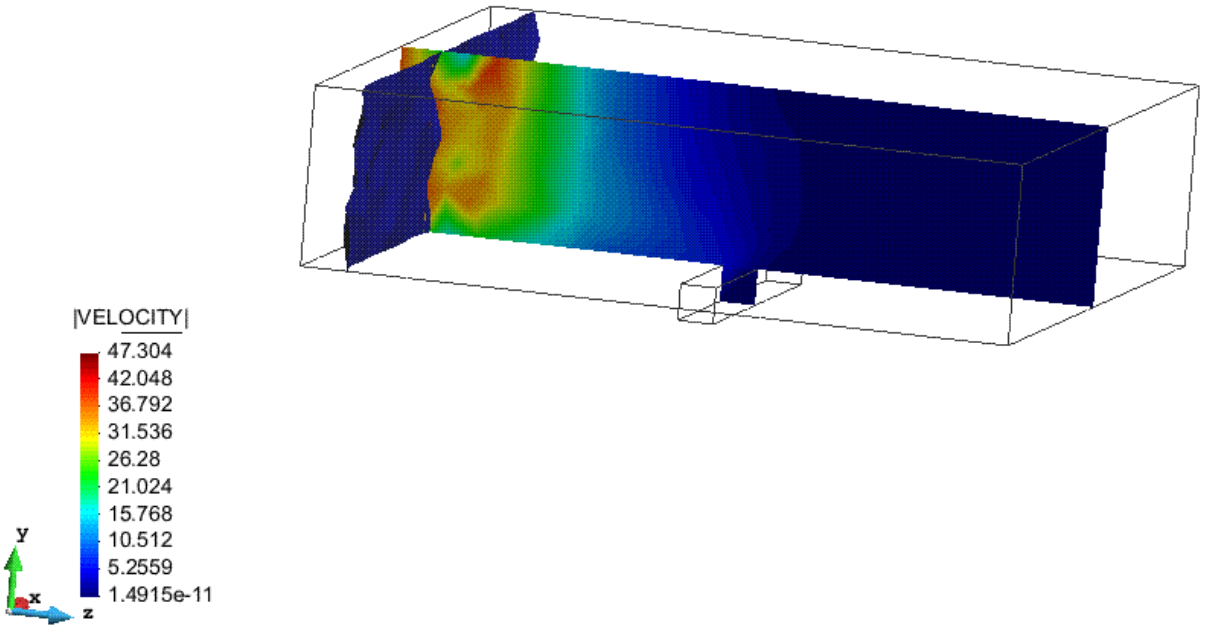
2.- Simulations of plastic injection at nano level

2.2 Fine mesh problematic



Air trap is detected on nano pools but also on fine mesh with flat surface

2.- Simulations of plastic injection at nano level
2.3 Submodelling approach



First simulation of submodelling without mesh transitions.
Boundary conditions to be improved with interpolation in position and time

2.- Simulations of plastic injection at nano level
2.4 Initial results

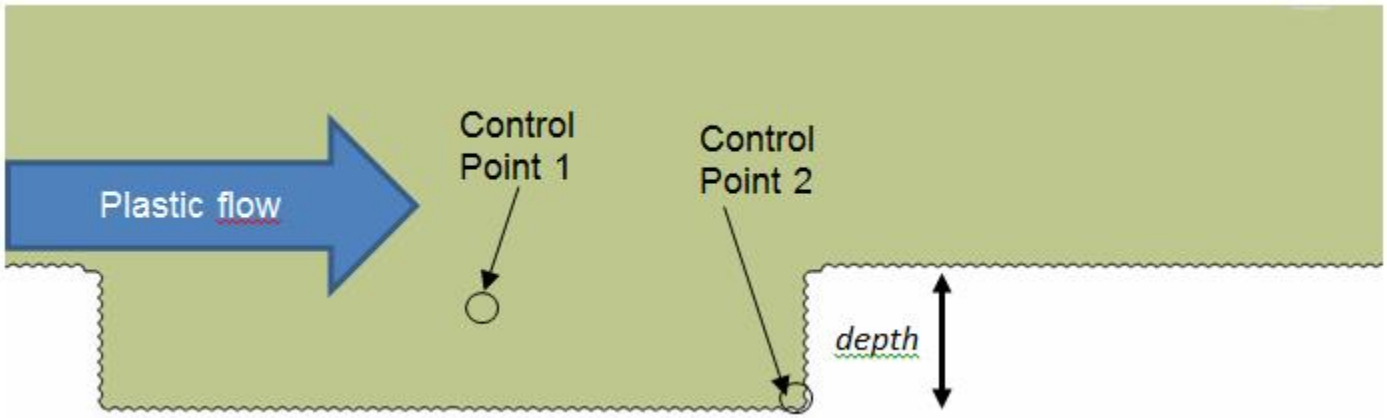
Several models are built to monitor roughness and other parameters for Polymer Replication on Nanoscale.

Combination of 2D and 3D models are used

With control points.

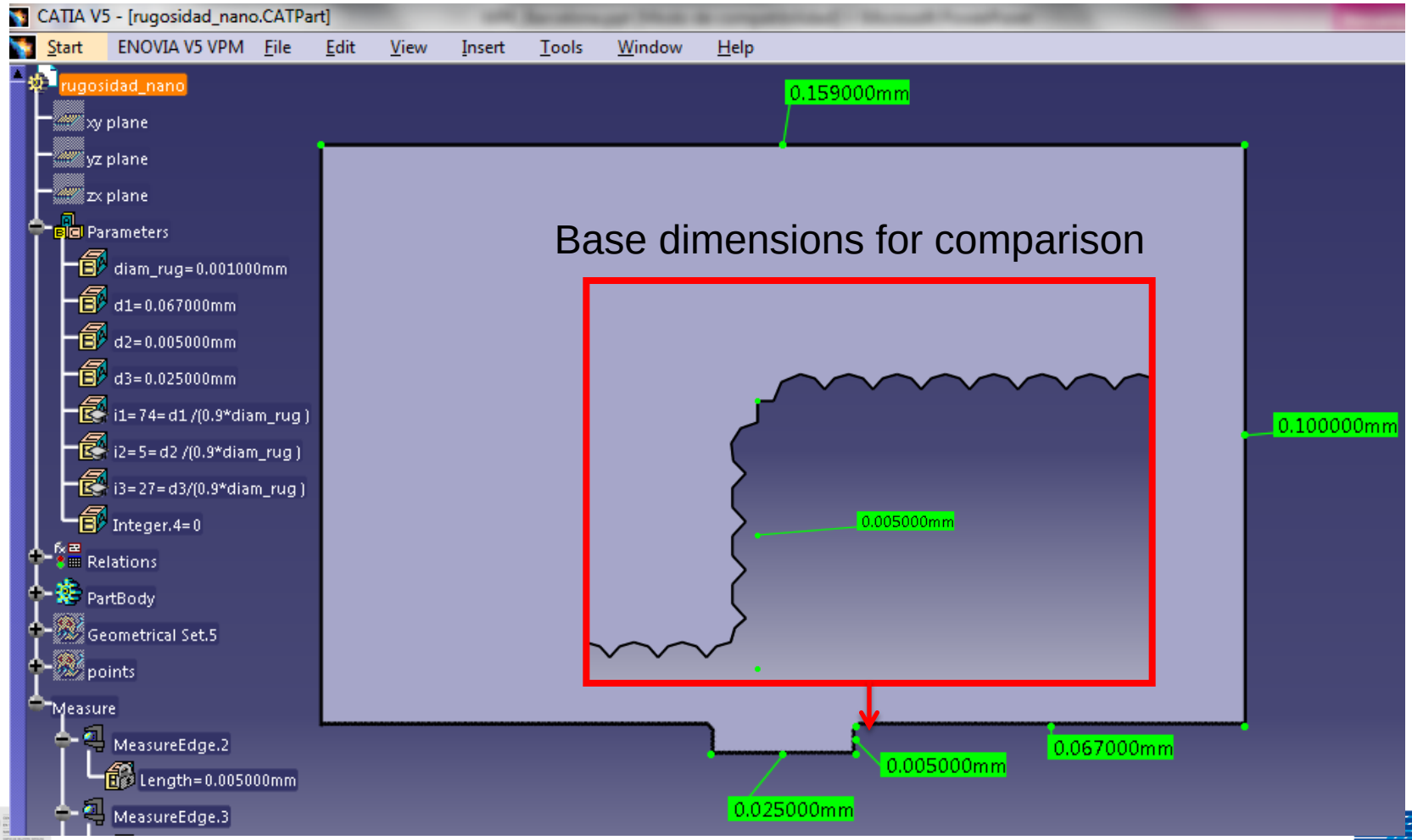
$$Ra = \frac{1}{n}\sum_{i=1}^{n}|z_i| \quad Rq = \sqrt{\frac{1}{n}\sum_{i=1}^{n} z_i^2}$$

$$Sq = \sqrt{\frac{1}{A}\iint_A z^2(x,y)\partial x \partial y}$$



2D simulation

2.- Simulations of plastic injection at nano level
2.4 Initial results



2.- Simulations of plastic injection at nano level
2.4 Initial results. Paremeters under study

Influence of roughness

Influence of velocity

Influence of pressures

Influence of nano pool length in radial direction.

Influence of nano pool width.

Influence of nano pool shape.

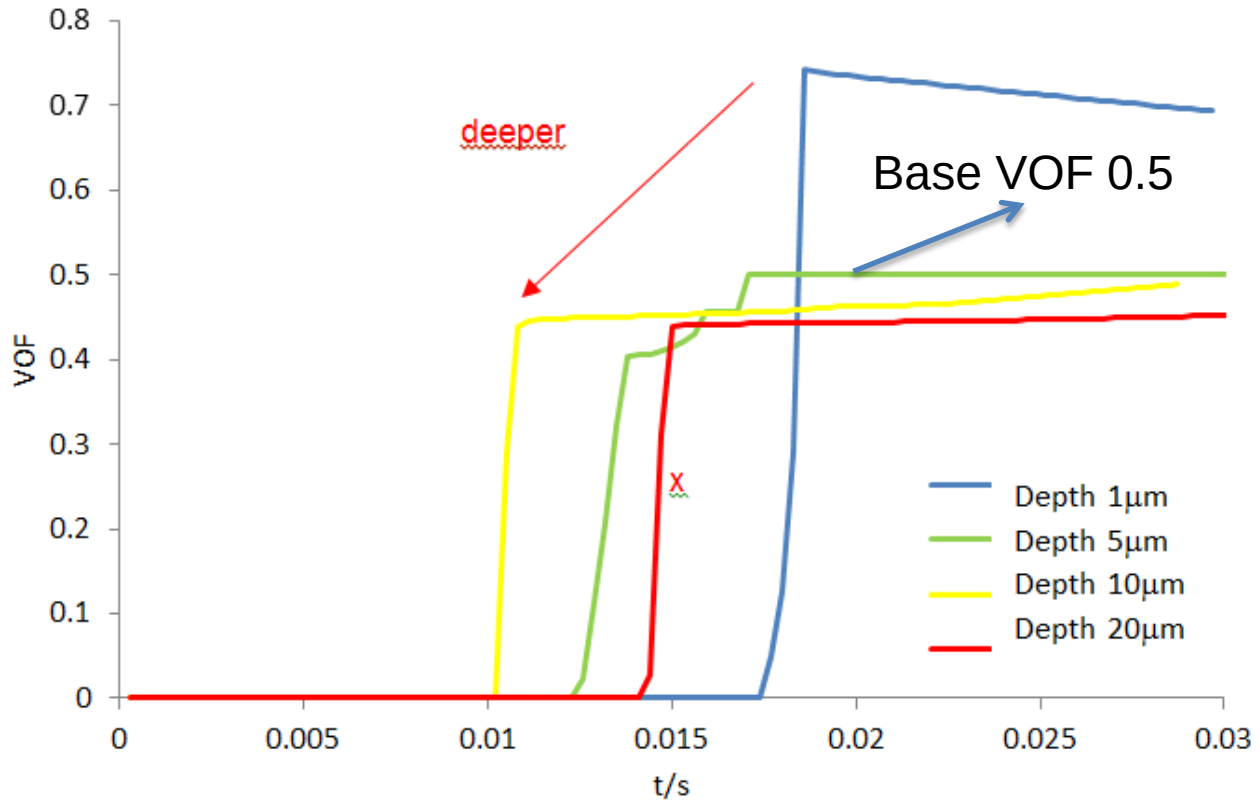
Influence of nano pool position next to each other in radial direction.

Influence of nano pool depth is explained next.

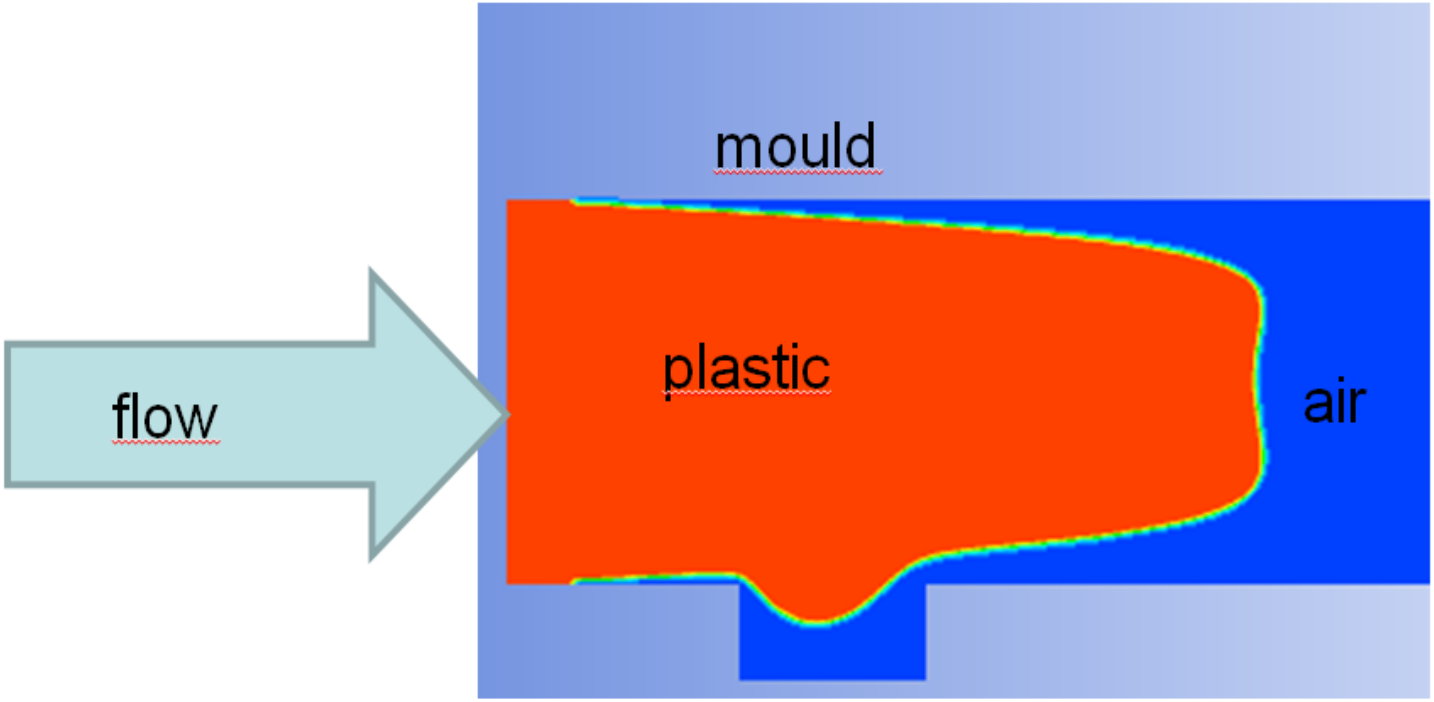
2.- Simulations of plastic injection at nano level
2.4 Initial results

Deeper nano pools fill worst with 0 roughness.

2D simulation



2.- Simulations of plastic injection at nano level
2.4 Initial results



3.- Experiments of plastic injection at nano level

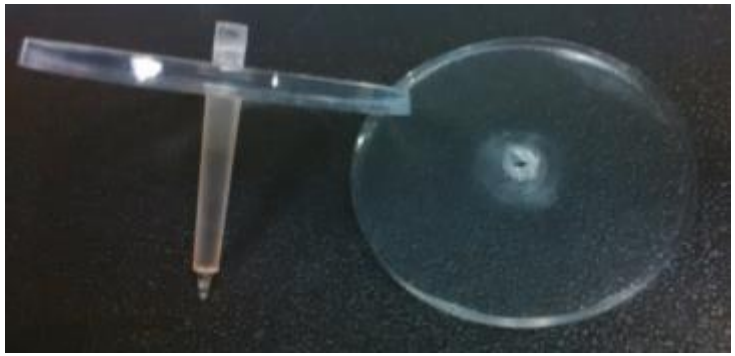
MOULD
Roughness
Micro pattern
Nano pattern

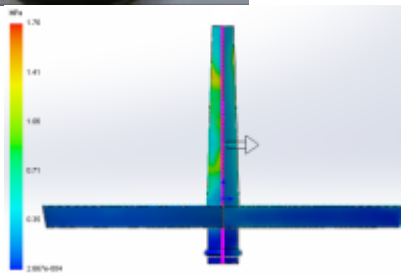
PLASTIC PART
Roughness?
Micro pattern?
Nano pattern?

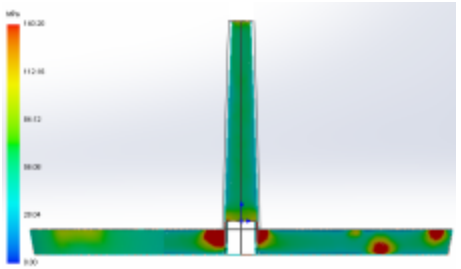
3.- Experiments of plastic injection at nano level

MOULD #1

MOULD #2

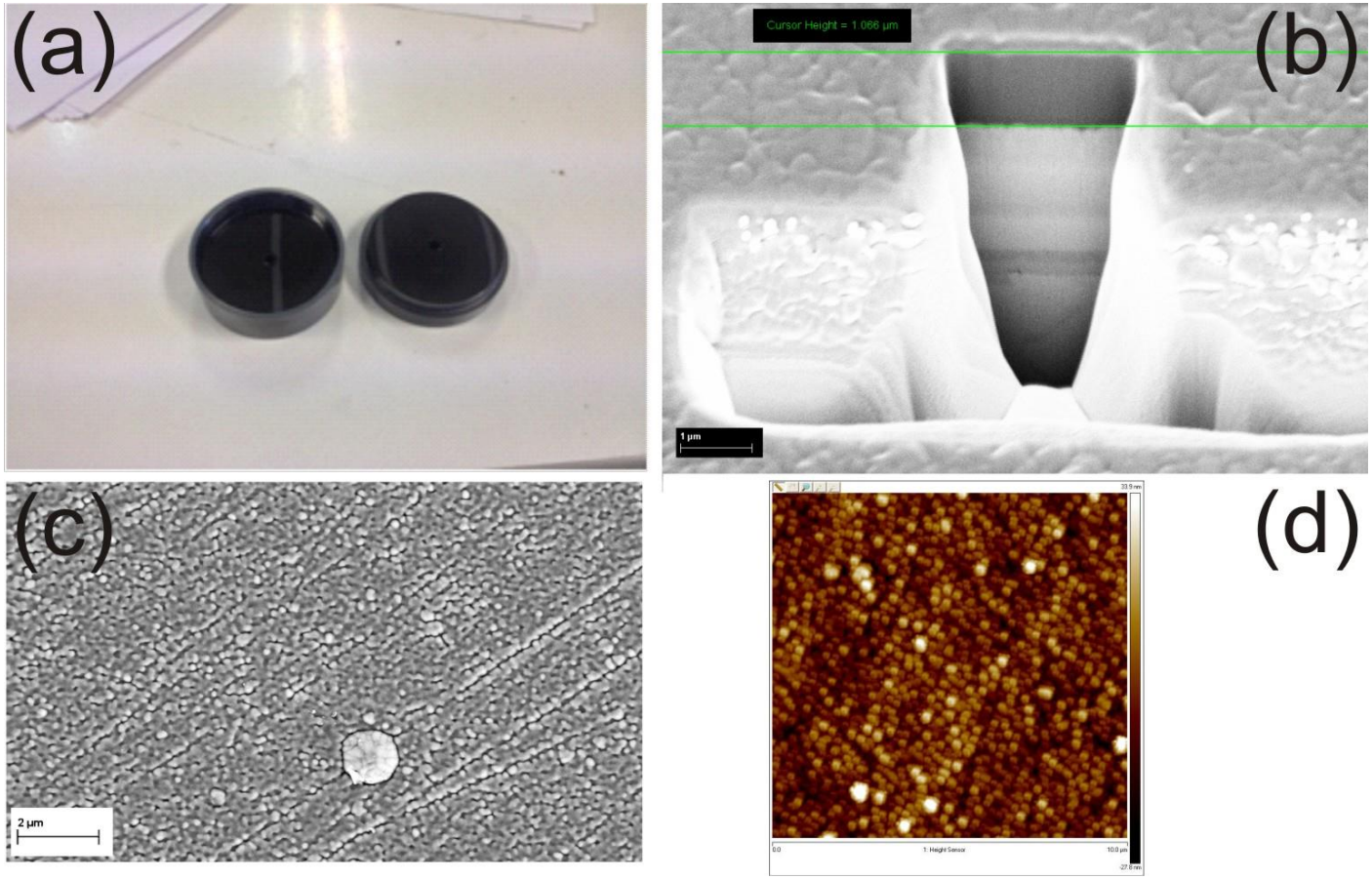






3.- Experiments of plastic injection at nano level

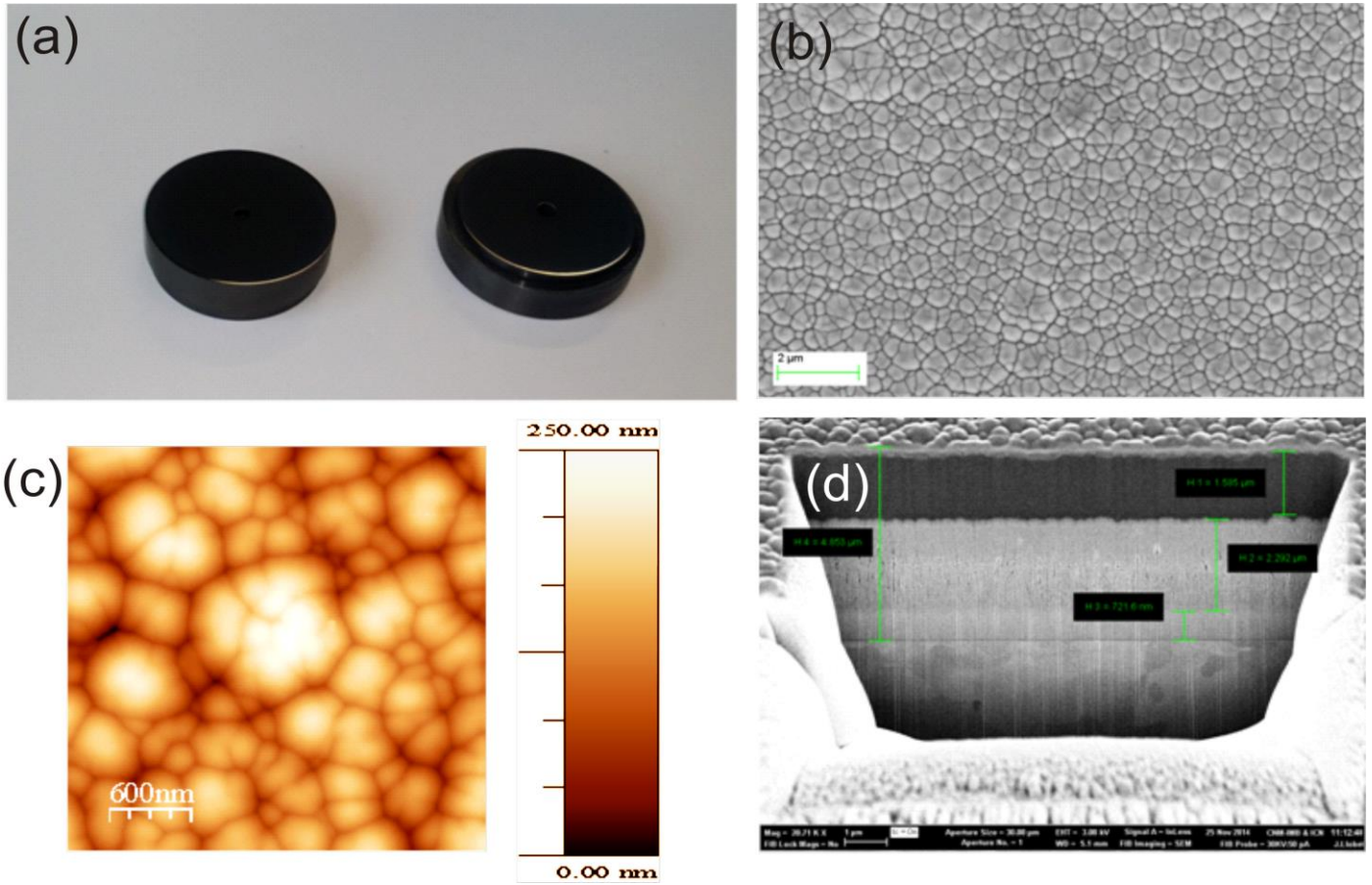
Mould #1 DLC coating



S_q c.a. 8 nm

3.- Experiments of plastic injection at nano level

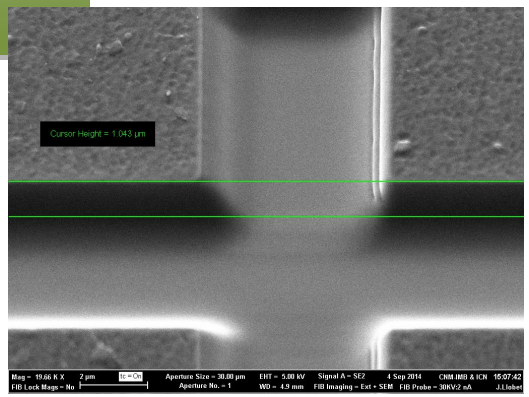
Mould #2 DLC coating

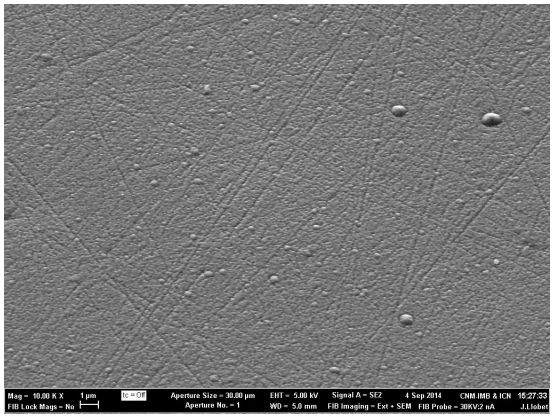


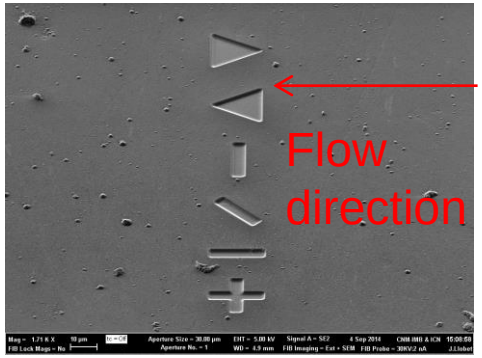
S_q c.a. 35 nm

3.- Experiments of plastic injection at nano level

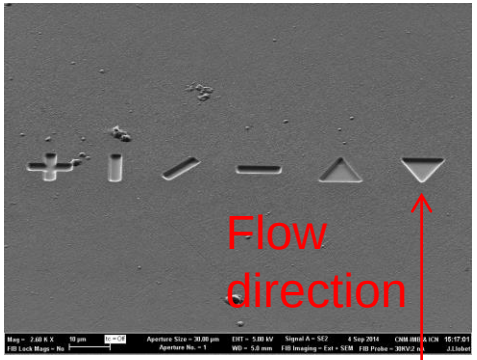
SEM images of the nano pools in mould #1



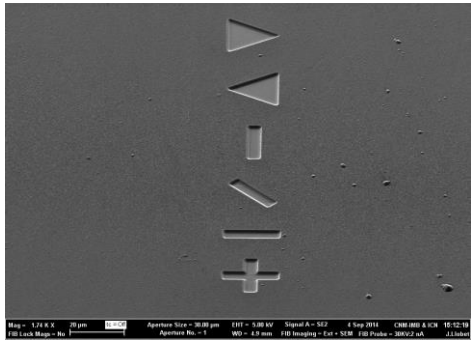




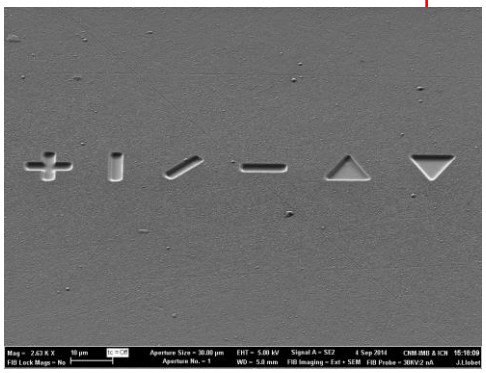
G1



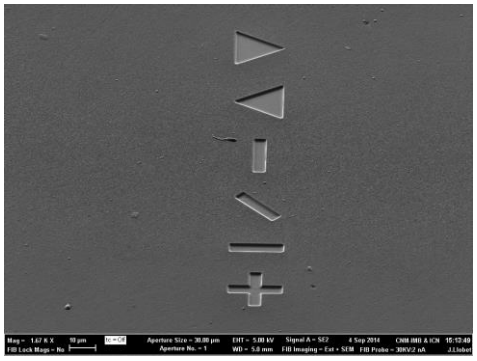
P1



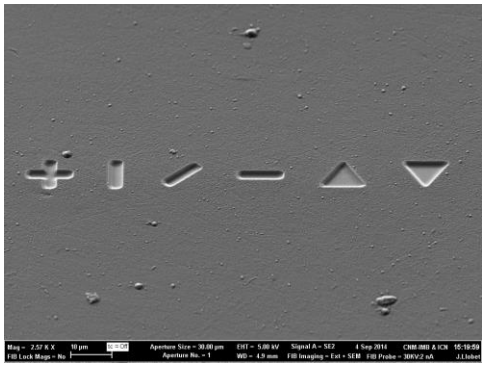
G2



P2

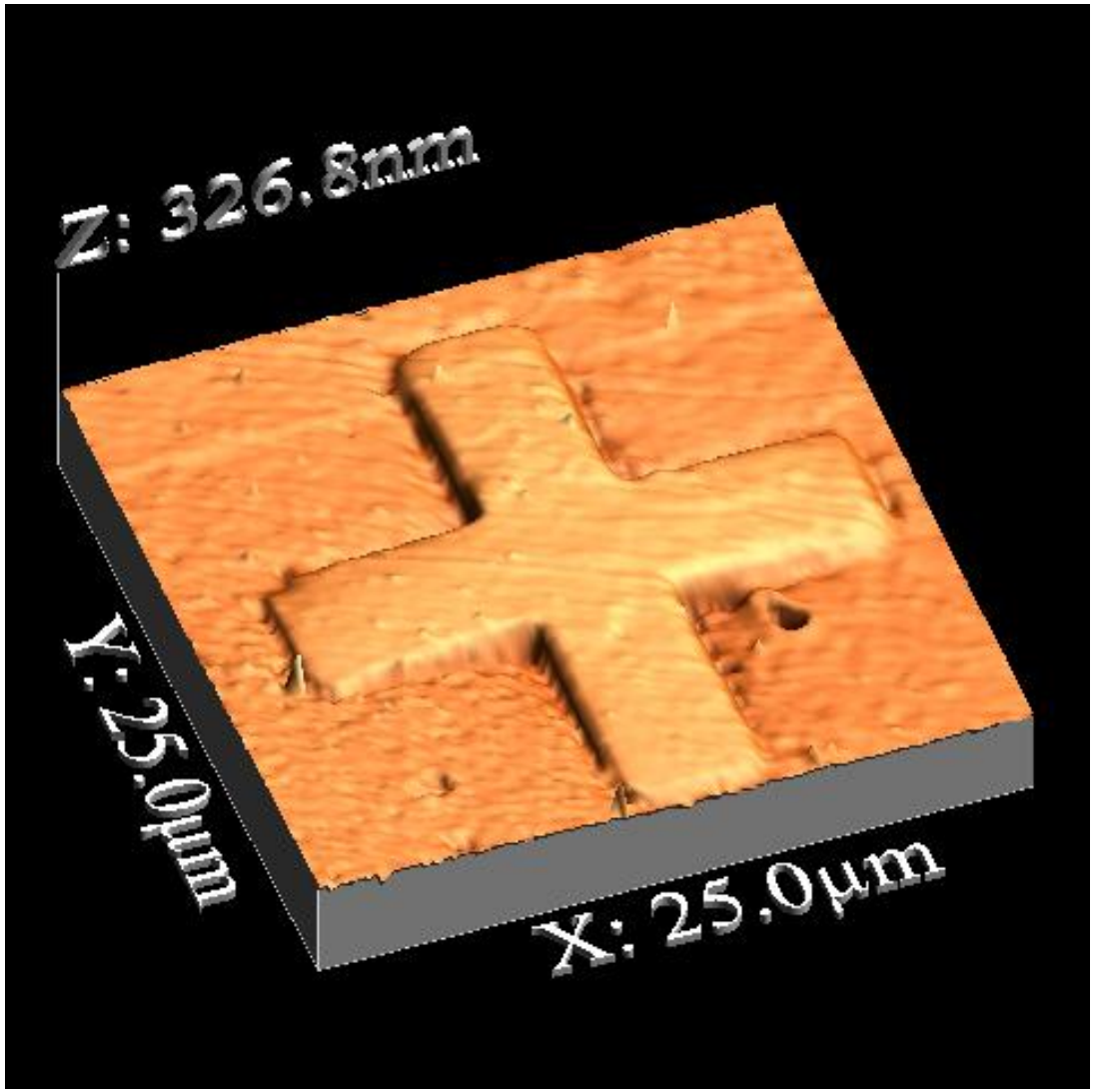


G3

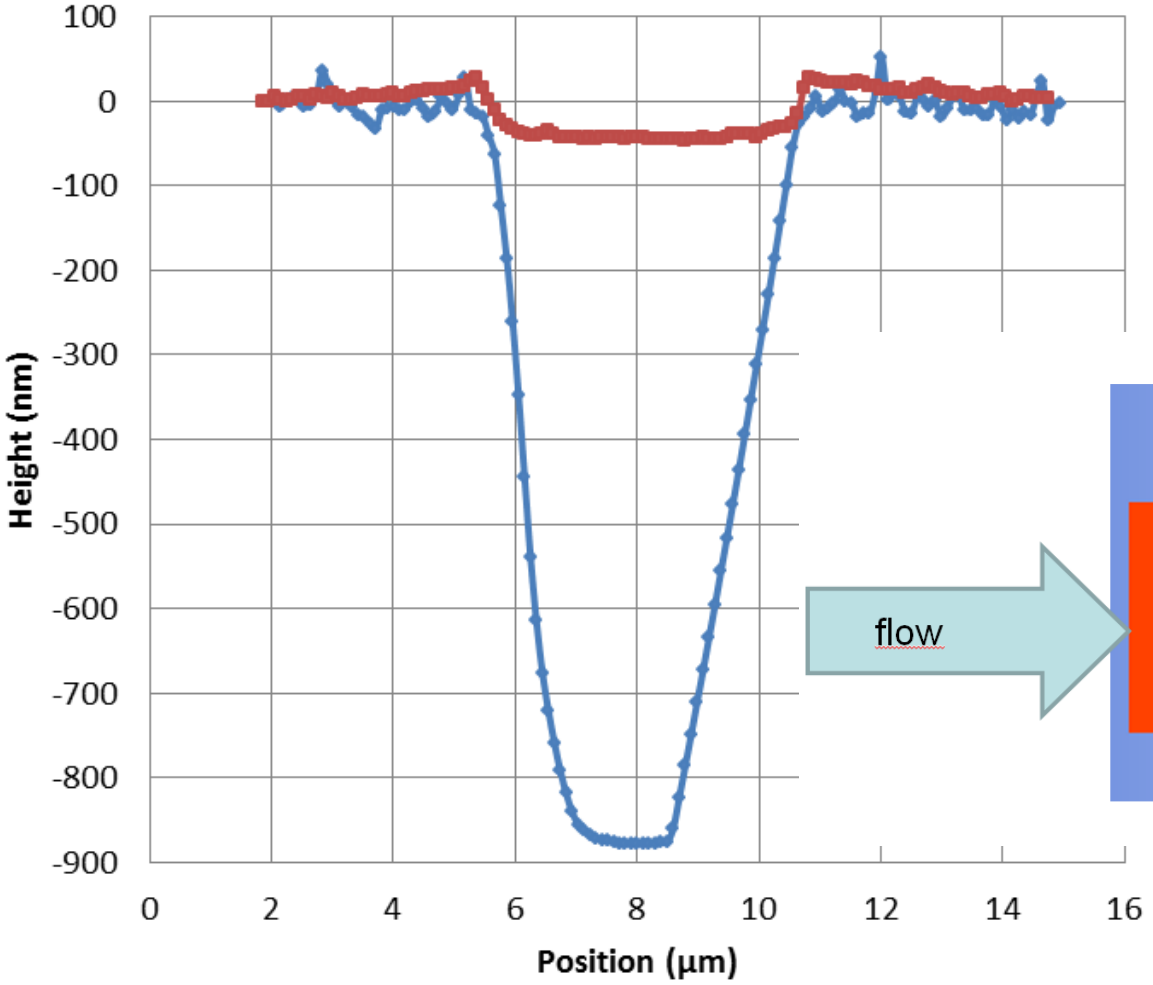


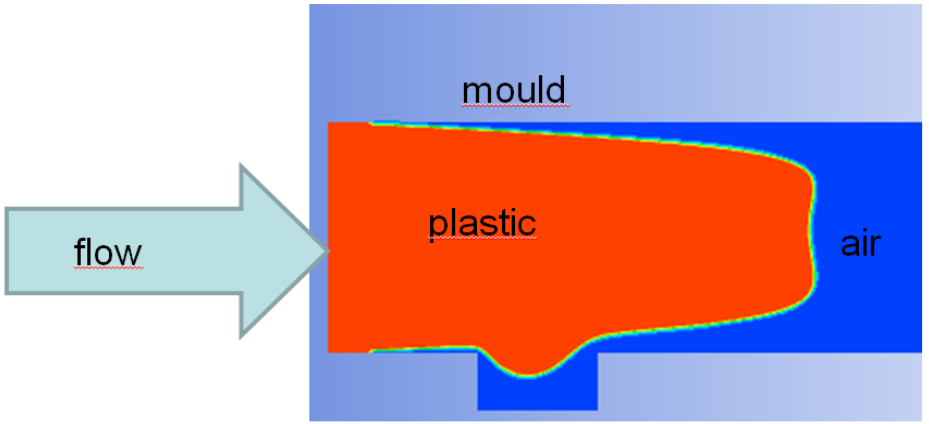
P3

3.- Experiments of plastic injection at nano level Replication on plastic parts



3.- Experiments of plastic injection at nano level

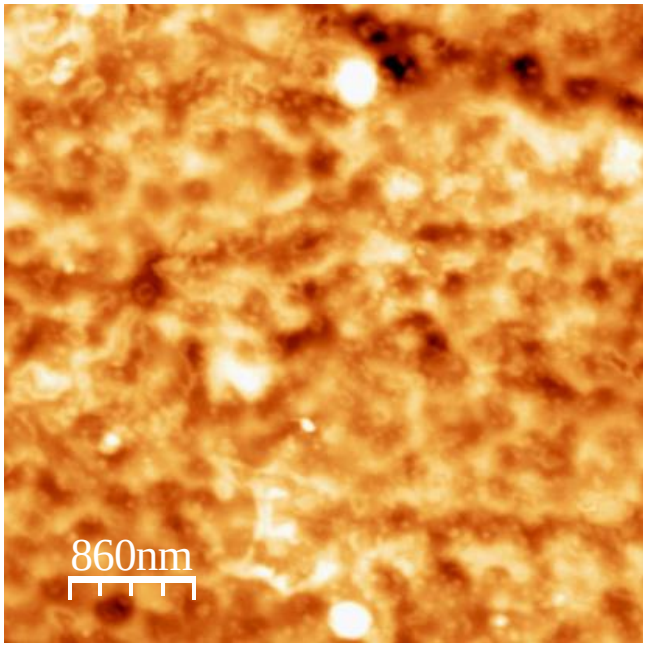




3.- Experiments of plastic injection at nano level
AFM images of marks in injected plastic pieces

STAMP

Roughness evaluation

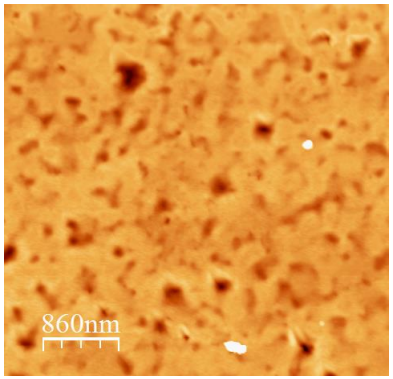


Ra: 4.815 nm
Sq: 6.3076 nm

INJECTED PLASTIC

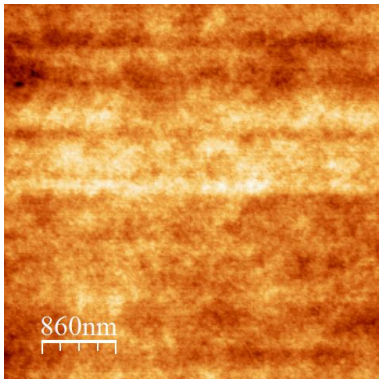
On substrate

Ra: 2.4934 nm
Sq: 3.9706 nm



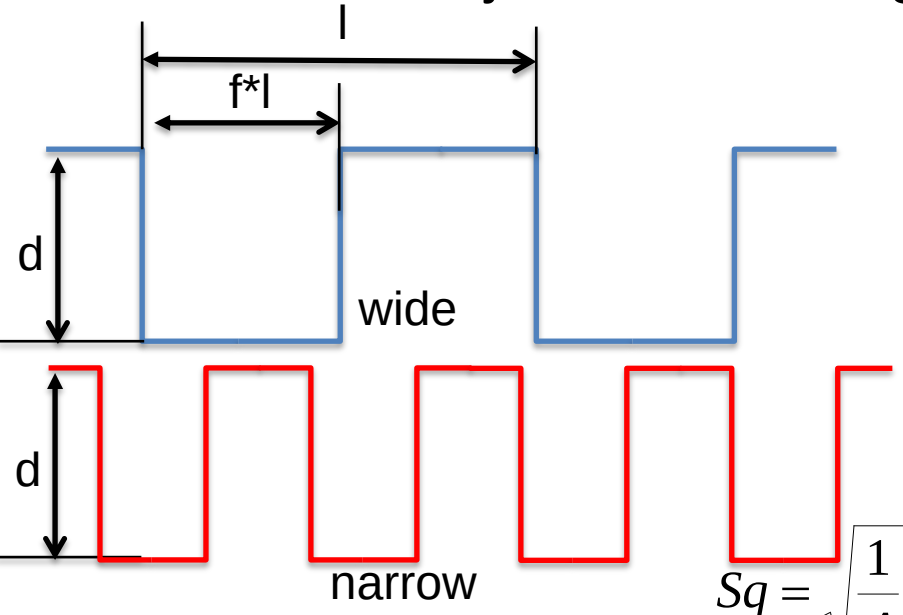
On marks

Ra: 0.4931 nm
Sq: 0.6178 nm



3.- SQ considerations for linear patterns

There are many surfaces with the same roughness leading to different injection moulding roughness.



$$Ra = \frac{1}{n}\sum_{i=1}^{n}|z_i| = d * f * (1-f) * 2$$

$$Ra_{(f\,0.5)} = 0.5 * d$$

$$Rq = \sqrt{\frac{1}{n}\sum_{i=1}^{n} z_i^2} = d\sqrt{f^2 * (1-f) + f * (1-f)^2}$$

$$Rq_{(f\,0.5)} = 0.5 * d$$

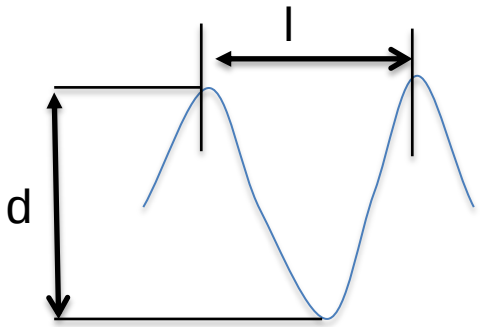
$$Sq = \sqrt{\frac{1}{A}\iint_A z^2(x,y)\partial x \partial y} = d\sqrt{f^2 * (1-f) + f * (1-f)^2}$$

$$Sq_{(f\,0.5)} = 0.5 * d$$

$$avg = (1-f) * d$$

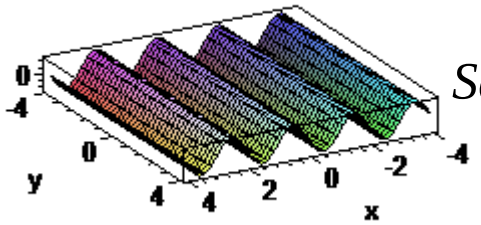
3.- SQ considerations for sinusoidal patterns

We can repeat the exercise for sinusoidal shapes in 2D and 3D:



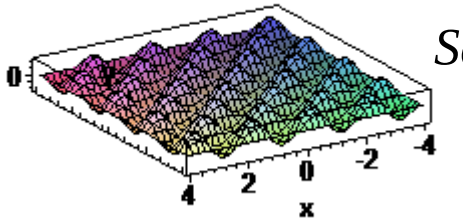
$$z_{2D} = \frac{d}{2}\sin\left(\frac{2\pi x}{l}\right)$$

$$Ra_{2D} = \frac{1}{L/2}\iint_A z(x,y)\partial x\partial y = d/\pi = 0.637 * d/2$$



$$Sq_{2D} = \sqrt{\frac{1}{A}\iint_A z^2(x,y)\partial x\partial y} = 0.7071 * d/2$$

$$z_{3D} = \frac{d}{2}\sin\left(\frac{2\pi x}{l}\right)\sin\left(\frac{2\pi y}{l}\right)$$



$$Sq_{3D} = \sqrt{\frac{1}{A}\iint_A z^2(x,y)\partial x\partial y} = 0.5 * d/2$$

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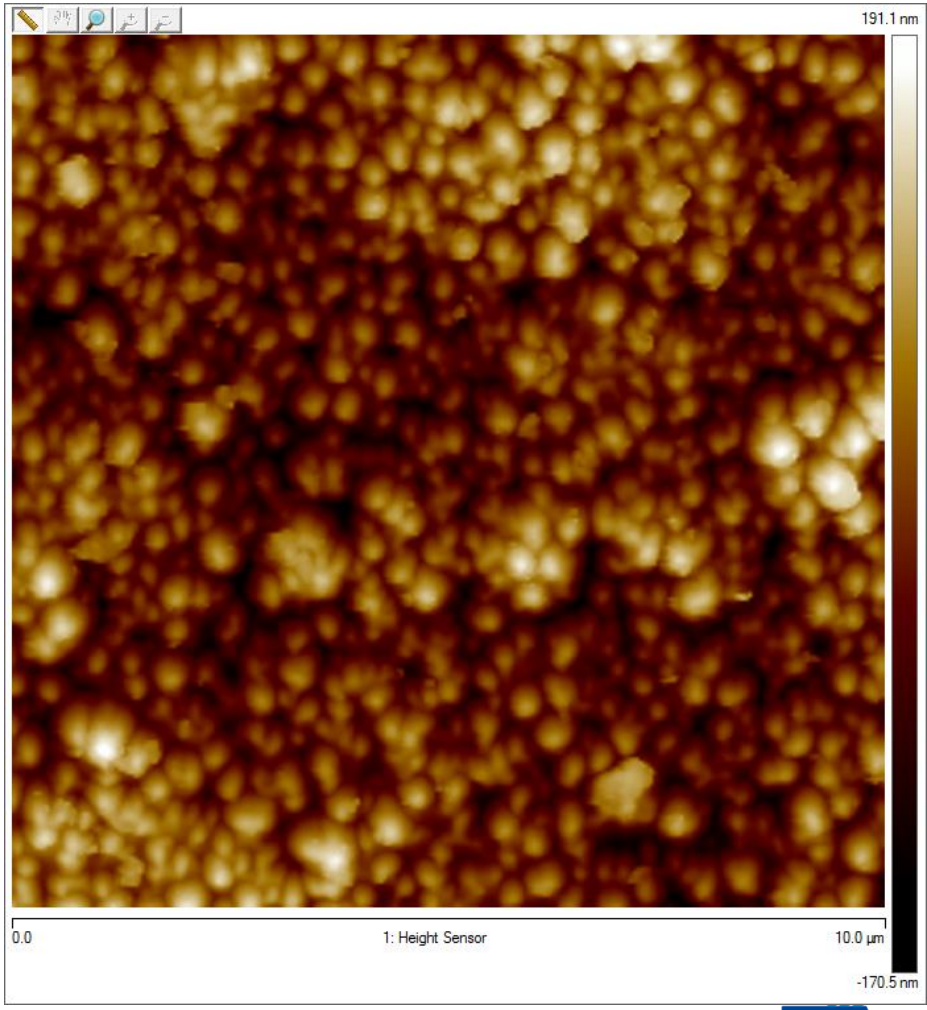
SEVENTH FRAMEWORK PROGRAMME

3.- Real topography

Real AFM topography:

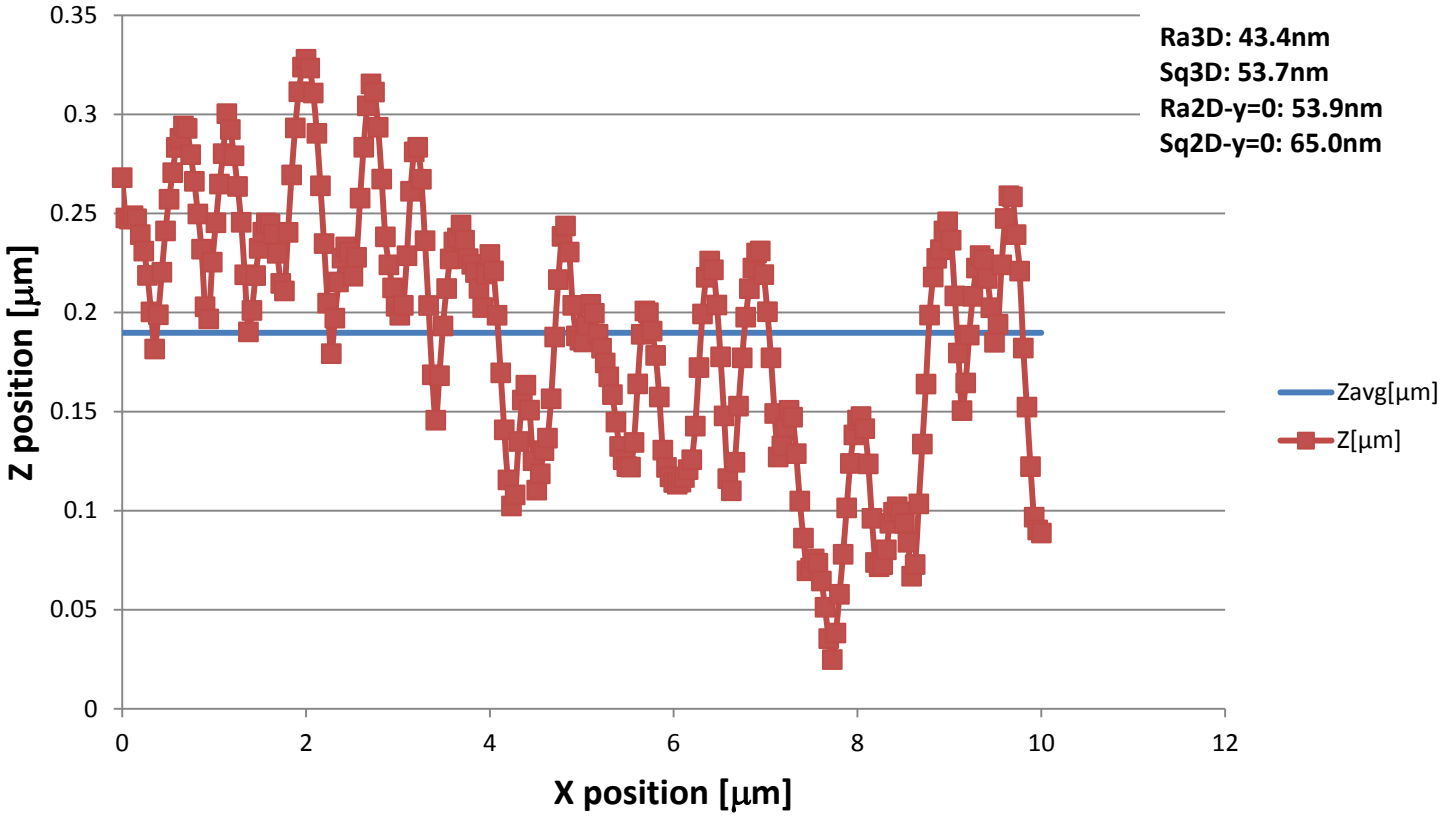
ELMAX

Rq=53.7 nm
Ra= 43.5 nm



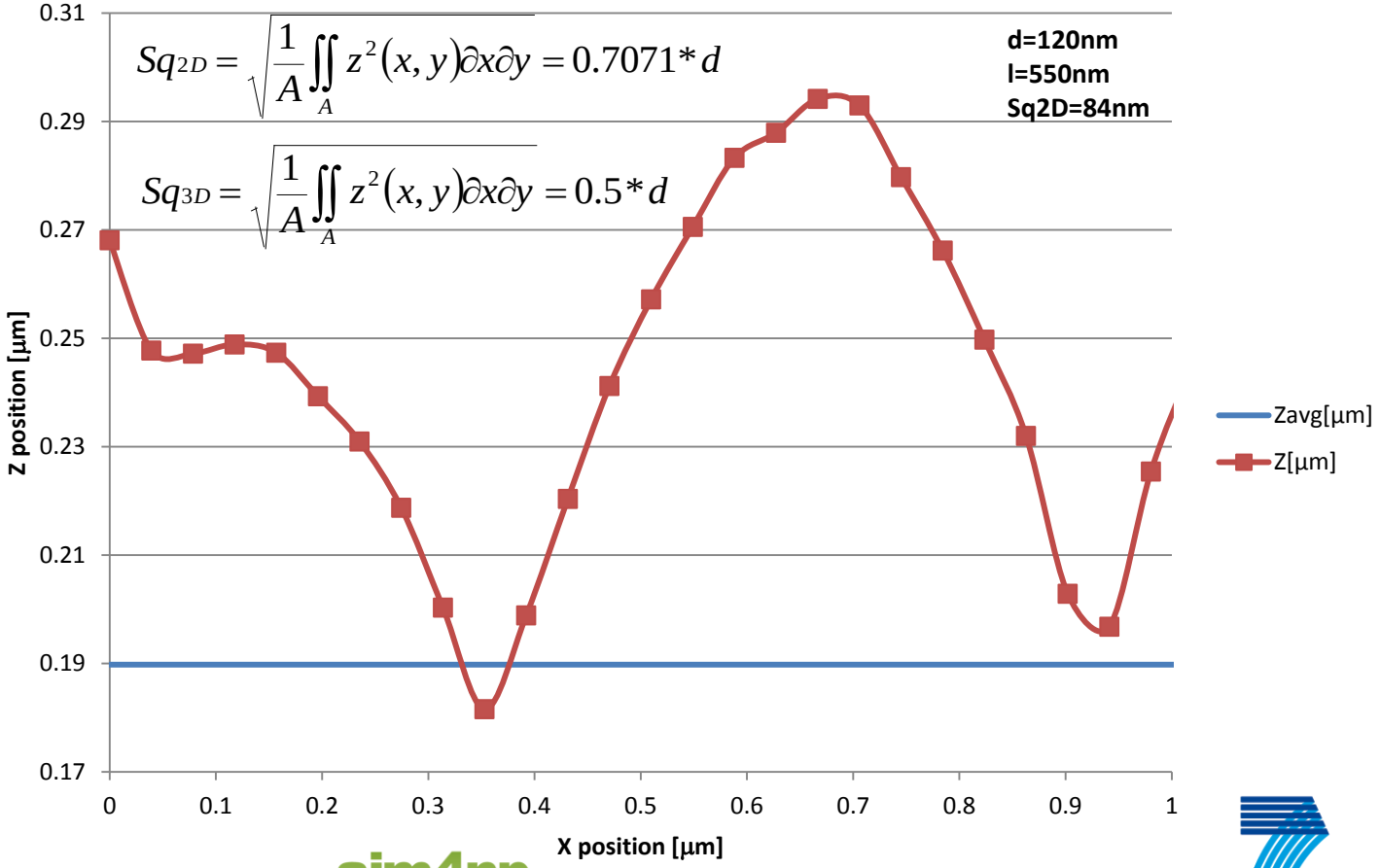
3.- Real topography

Real AFM topography with Excel for simulation y=0:



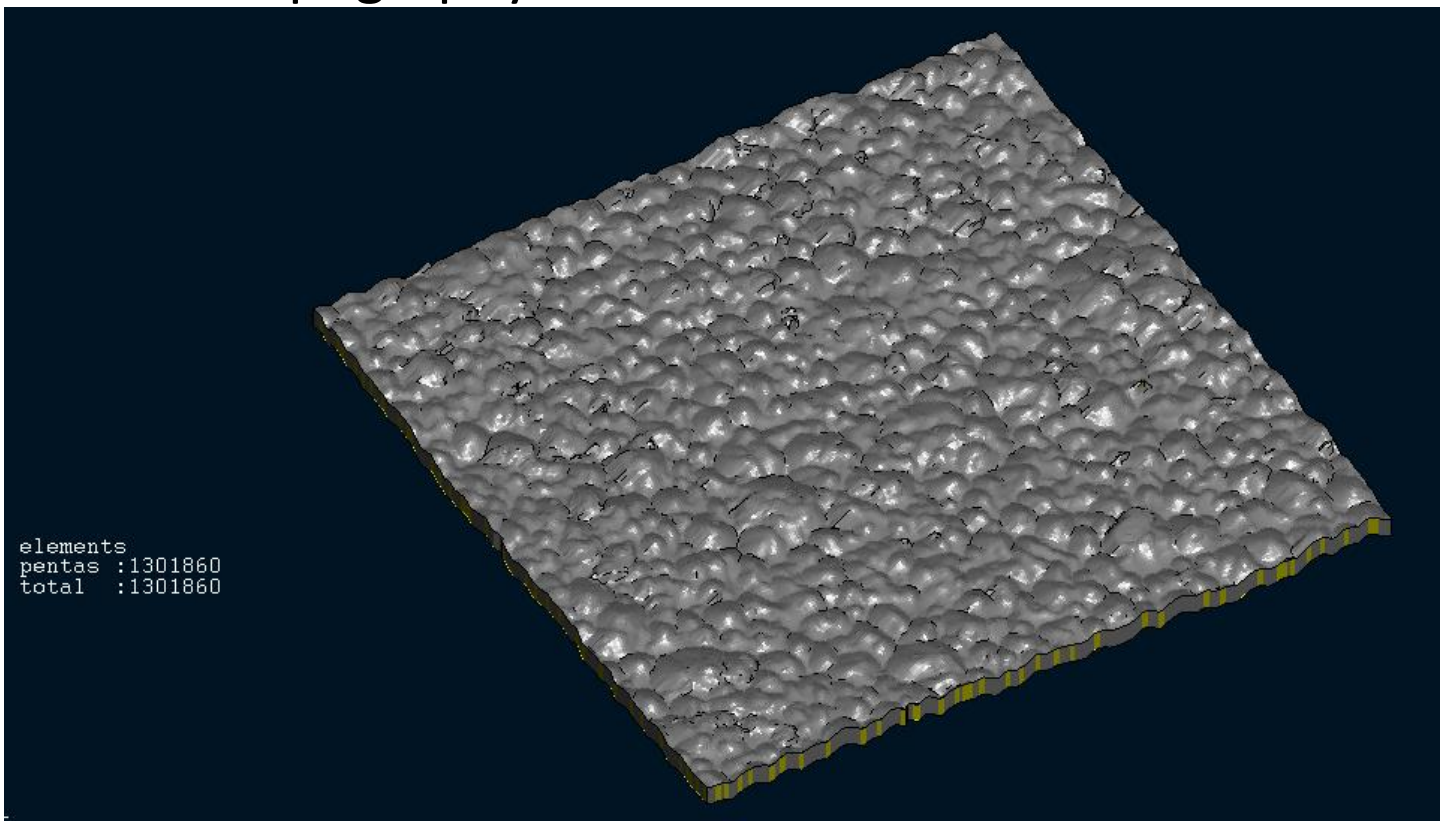
3.- Real topography

Real AFM topography with Excel for simulation small area y=0, x(0,1):



3.- Real topography

Real AFM topography inside simulation software:

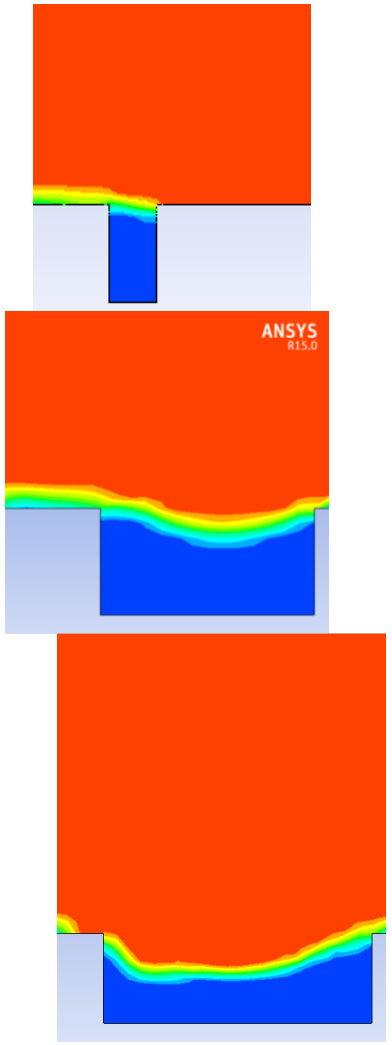


3.- Previous simulations for correlation

Previous simulations for several roughness playing with width for a single mark. Depth was set to 100nm and width was used from 50nm to 300nm.

Sq with a single mark can not be calculated:

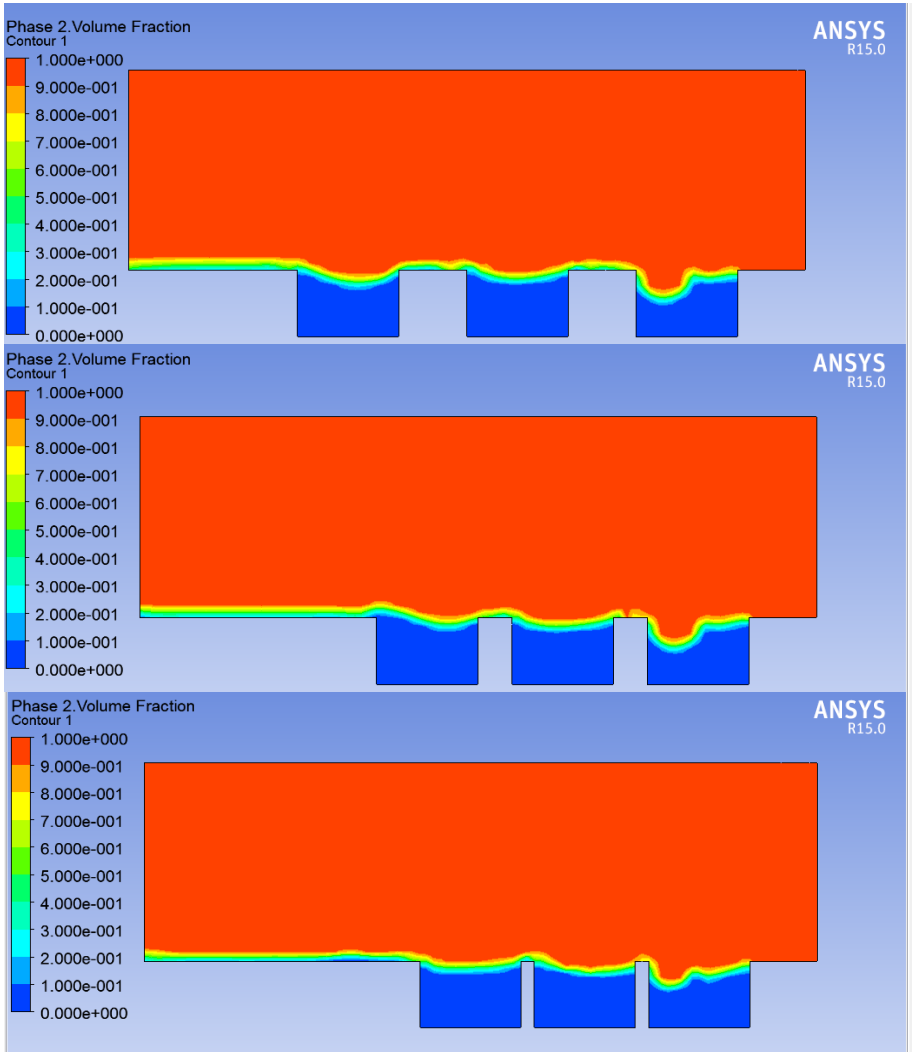
$$Sq = \sqrt{\frac{1}{A}\iint_A z^2(x,y)\partial x \partial y} = d\sqrt{f^2 * (1-f) + f * (1-f)^2}$$



3.- Previous simulations for correlation

Simulations for several roughness playing with parameter “f”

f	Sq
0.4	0.489898
0.25	0.433013
0.117647	0.32219



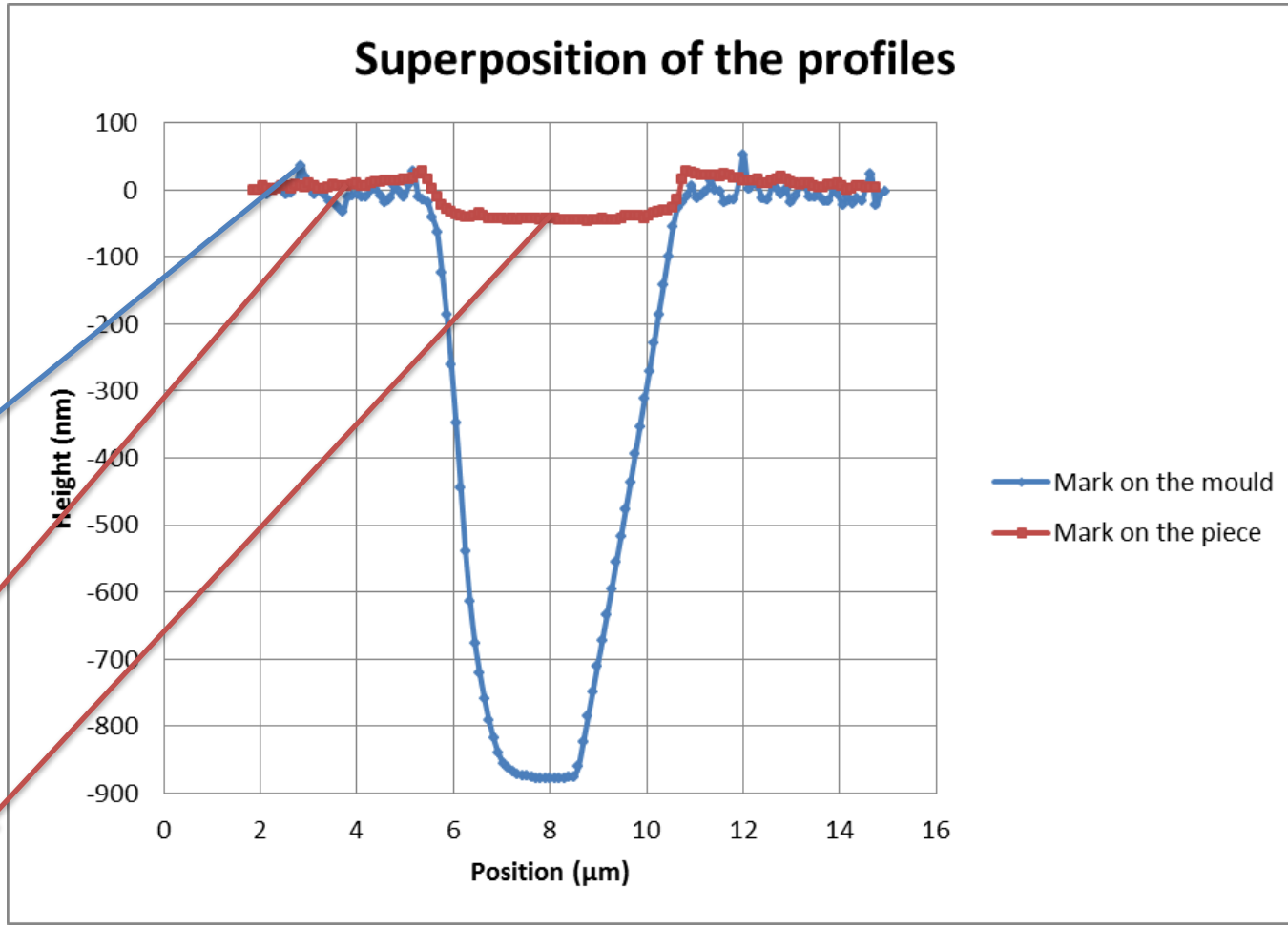
3.- Real topography mould and plastic

Experienced gained.

Mould
Ra: 4.815 nm
Sq: 6.3076 nm

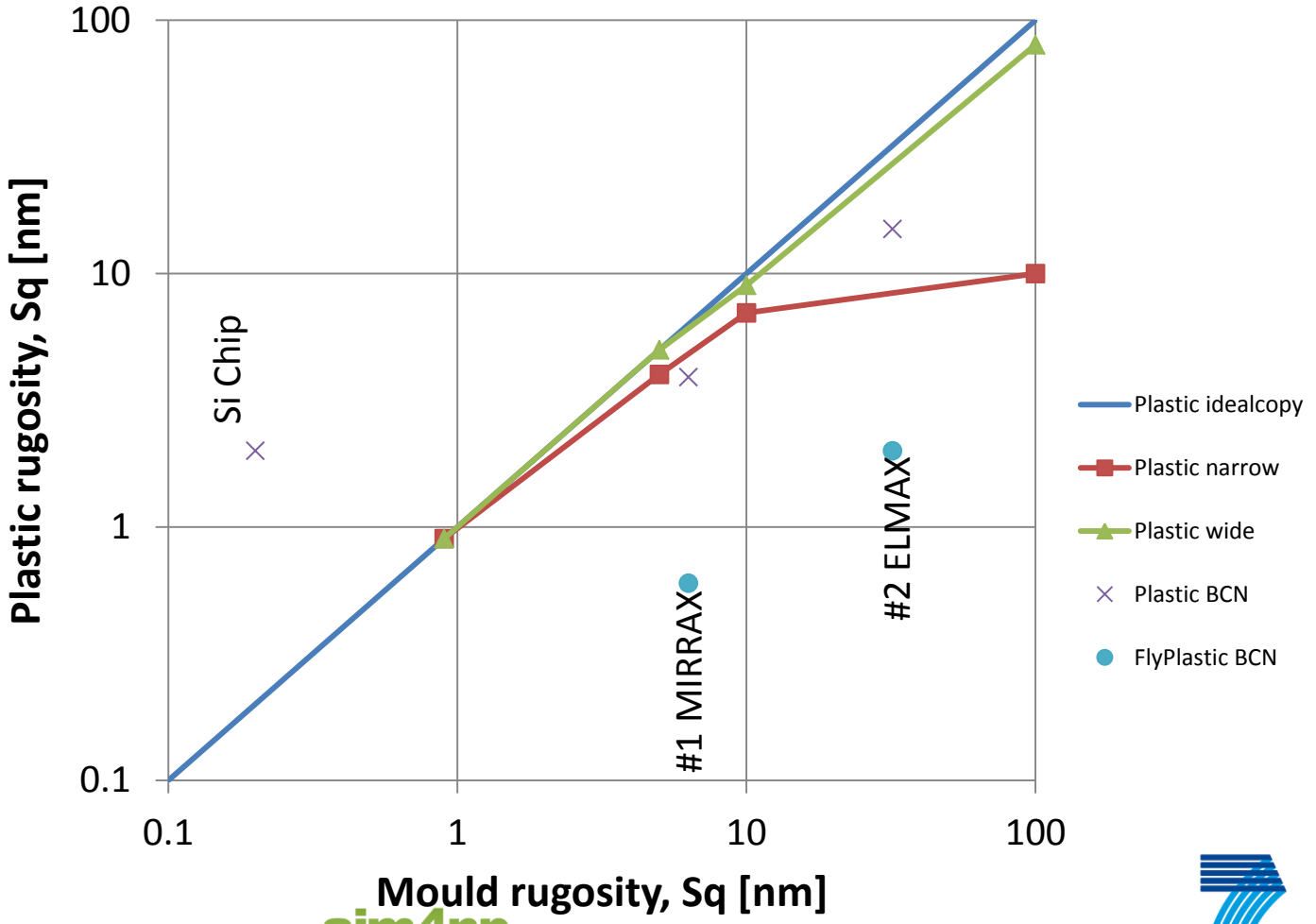
Plastic:
Ra: 2.4934 nm
Sq: 3.9706 nm

Fly-plastic:
Ra: 0.4931 nm
Sq: 0.6178 nm



3.- Simulations and measurements for roughness prediction

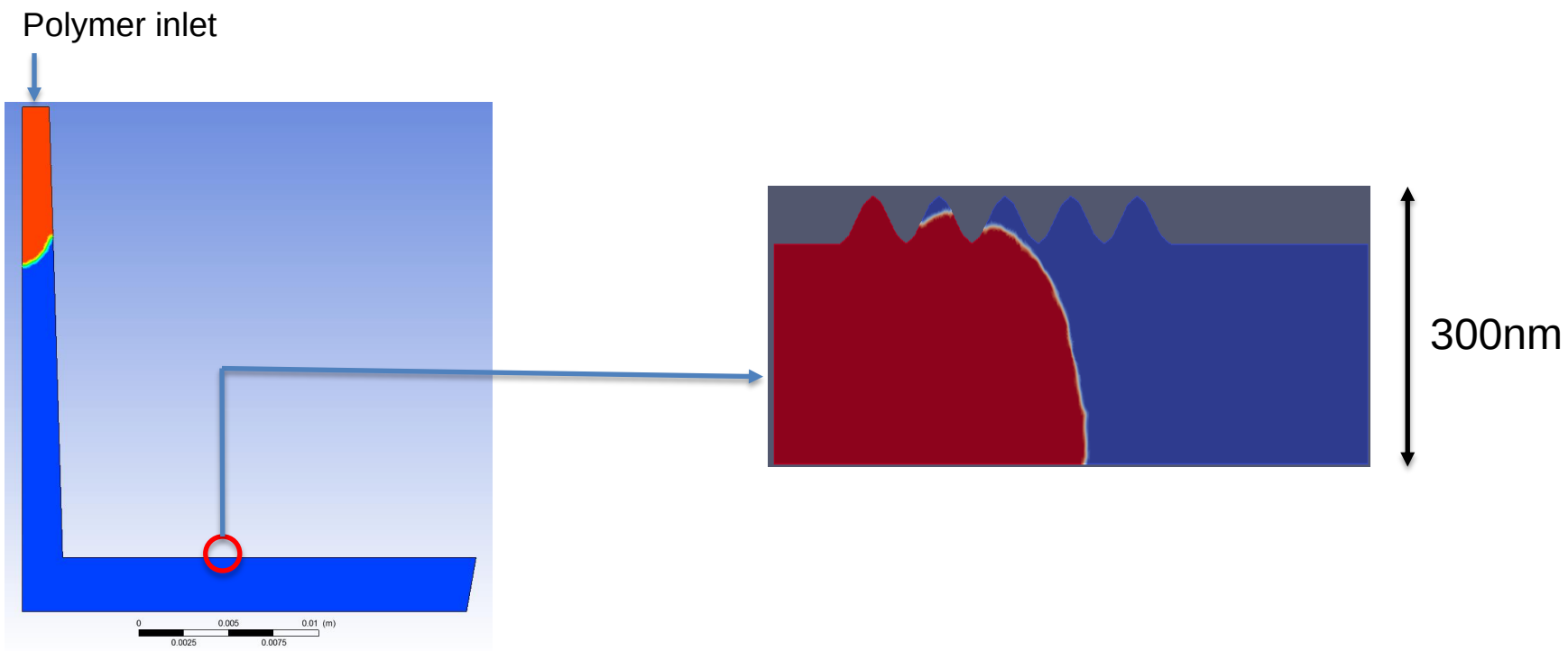
Expected behaviour



3.- Simulations and measurements for roughness prediction

How not? Nanomesh in whole model or mesh refining

How yes? Submodeling

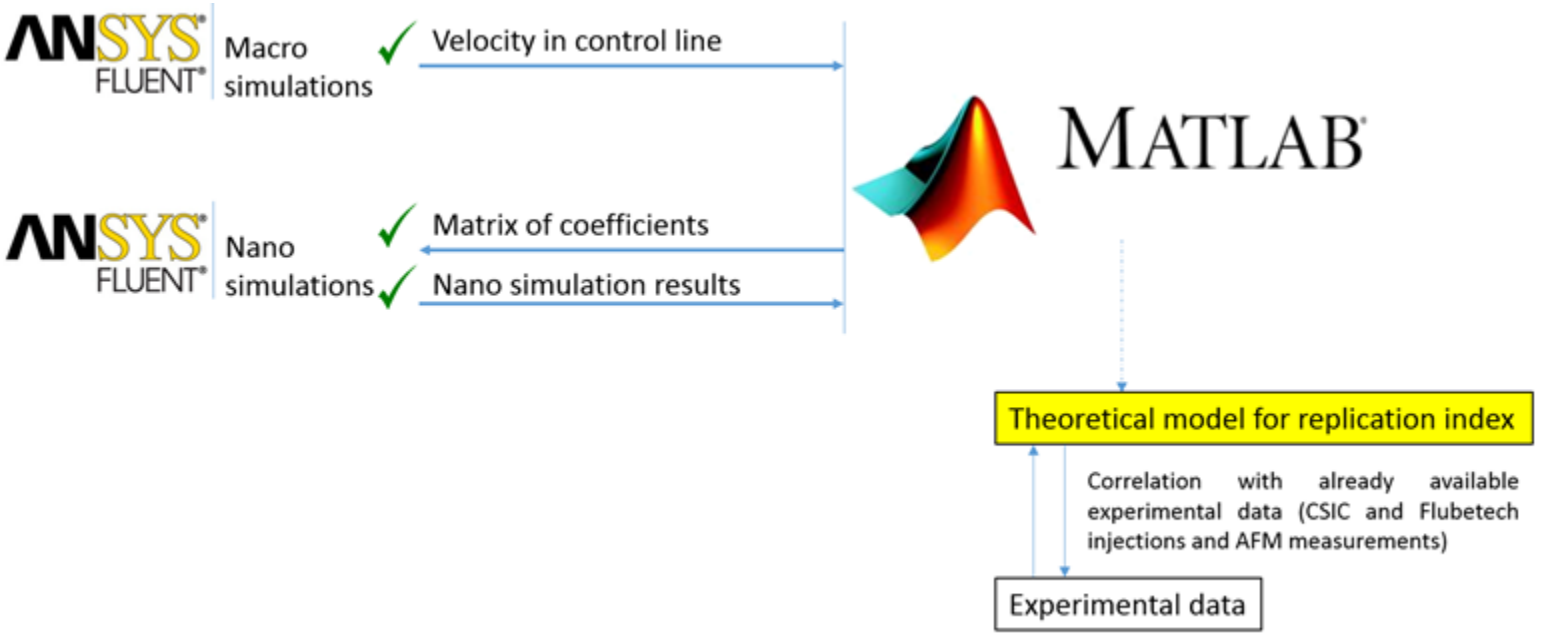


Macro simulation

Nano simulation

3.- Simulations and measurements for roughness prediction

Procedure

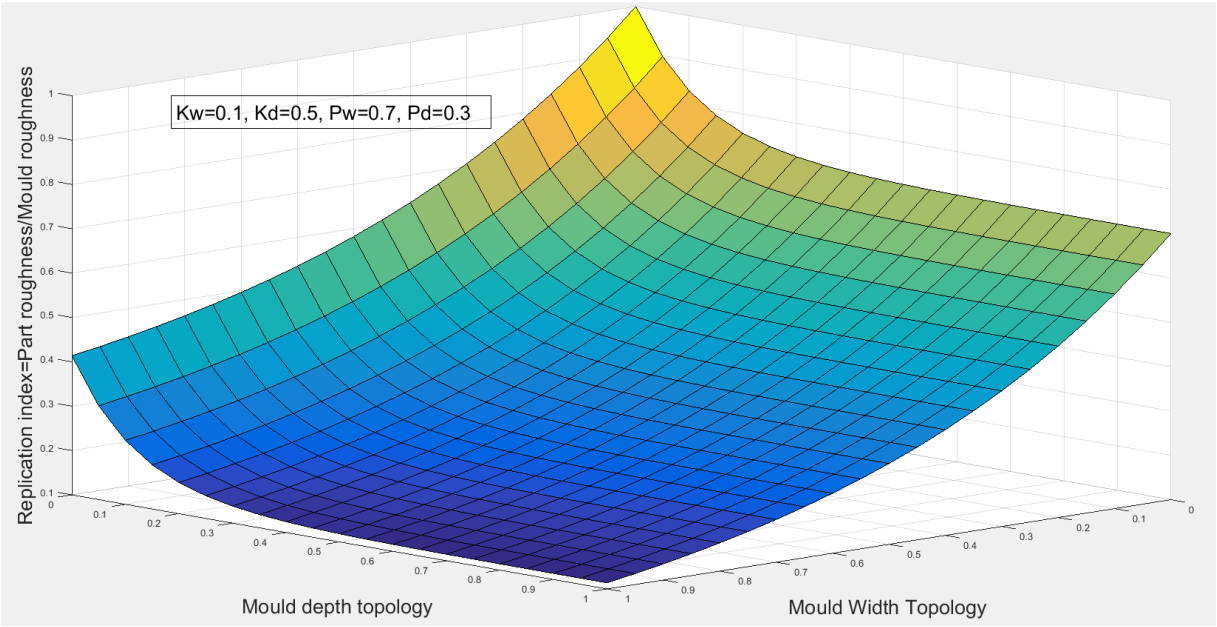


3.- Simulations and measurements for roughness prediction

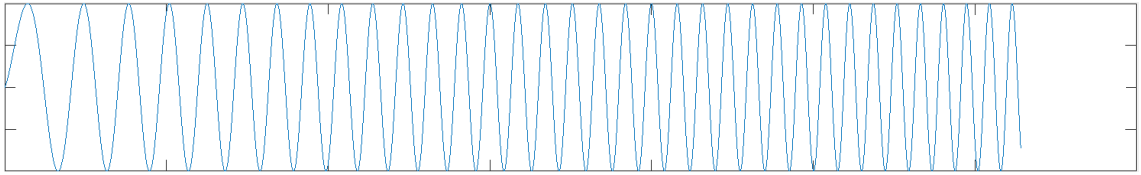
First model

$$RI = P_w e^{\frac{-W}{K_w}} + P_d e^{\frac{-D}{K_d}}$$

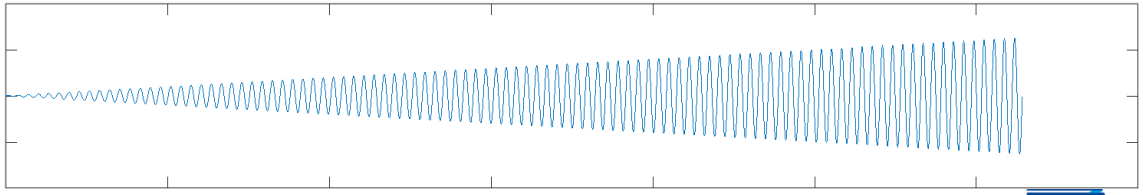
$$P_w + P_d = 1$$



Mould width topology

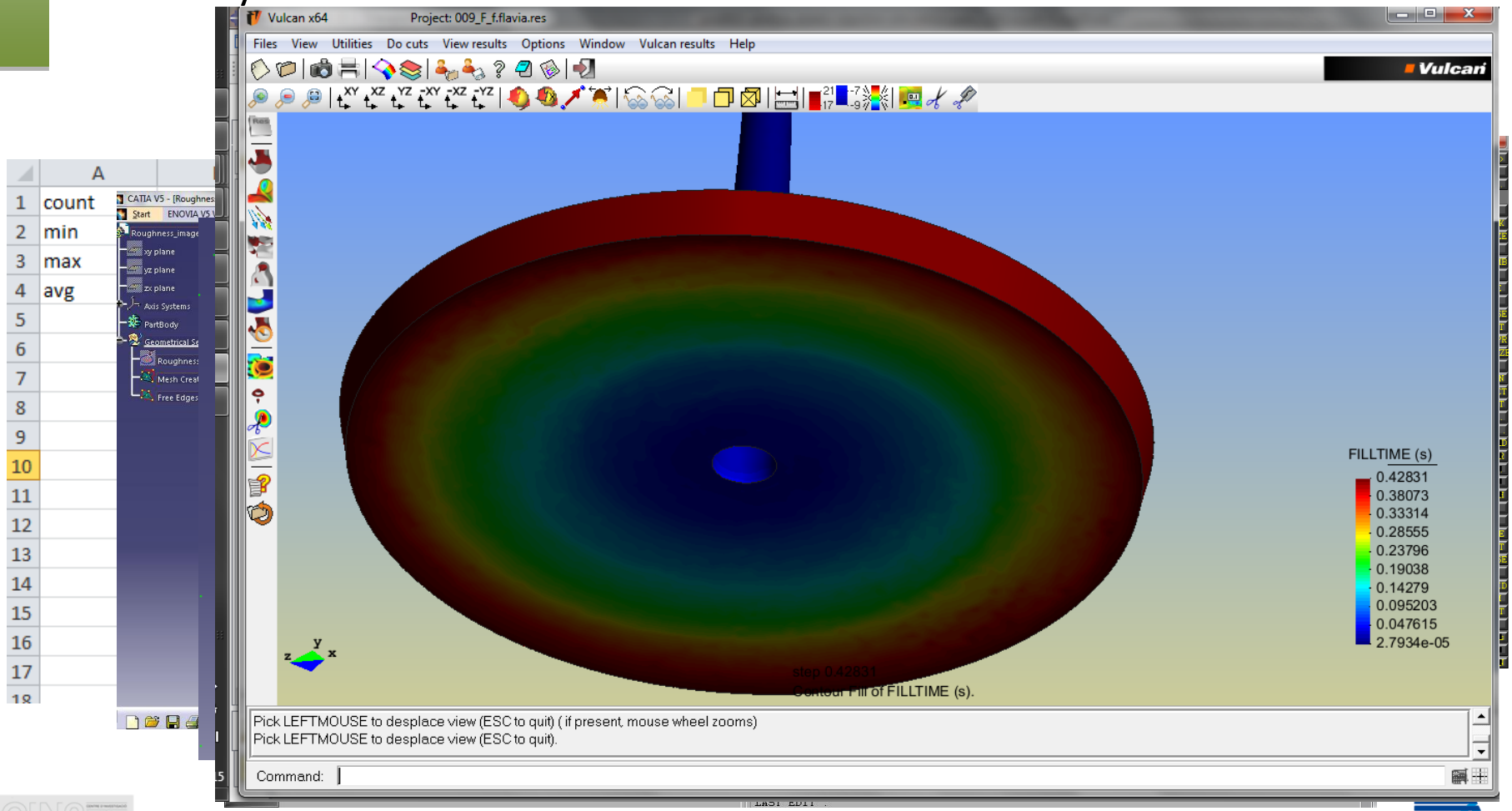


Mould depth topology



4.- Next steps

- Improve submodelling technique for automation of interpolation in position and time of boundary conditions.
- Carry out simulations with AFM



THANK YOU