PRN 2015 Simulation of plastic injection for nanostructure pattern replication Copenhagen, 19<sup>th</sup> May 2015

J.Pina-Estany<sup>1</sup>, J.Fraxedas<sup>3</sup>, F.Perez-Murano<sup>3</sup>, C.Colominas<sup>2</sup>, J.M.Puigoriol-Forcada<sup>1</sup>, A.A.Garcia-Granada<sup>1</sup>

<sup>1</sup>IQS-Universitat Ramon Llull; <sup>2</sup>Flubetech SL; <sup>3</sup>ICN2-CNM-CSIC Barcelona;

Contact: andres.garcia@iqs.edu, Via Augusta 390, E08017, Barcelona, Spain.







### 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!



<u>aim4np</u>

### 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



### 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</li>
  - actuation range)

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



# 1.- Introduction to aim4np projectPlastic 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.











### 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 level2.1 Model to validate

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



## 2.- Simulations of plastic injection at nano level2.2 Fine mesh problematic



2.654e-004









# 2.- Simulations of plastic injection at nano level2.2 Fine mesh problematic



Shear stress and Volume shrinkage around control nano pool







# 2.- Simulations of plastic injection at nano level2.2 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 level2.3 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 level2.4 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.  $Sq = \sqrt{\frac{1}{A} \iint_{i=1}^{n} z^{2}(x, y) \partial x \partial y}$ 



## 2.- Simulations of plastic injection at nano level2.4 Initial results



# 2.- Simulations of plastic injection at nano level2.4 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 level2.4 Initial results

Deeper nano pools fill worst with 0 roughness.

0.8

0.7 deeper Base VOF 0.5 0.6 2D simulation 0.5 ច្<u>ខ</u> 0.4 0.3 Depth 1µm 0.2 Depth 5µm Depth 10µm 0.1 Depth 20µm 0 0.005 0.02 0.025 0.03 0.01 0.015 0 t/s aim4np 21 ne SEVENTH FRAMEWORK PROGRAMME

## 2.- Simulations of plastic injection at nano level2.4 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



CSIC

### 3.- Experiments of plastic injection at nano level Mould #2 DLC coating





S<sub>q</sub> c.a. 35 nm





#### 3.- Experiments of plastic injection at nano level

direction

#### SEM images of the nano pools in mould #1





hei





27

SEVENTH FRAMEWORK

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









#### 3.- Experiments of plastic injection at nano level



Flube

IQ

Universitat Ramon Llull

SEVENTH FRAMEWORK PROGRAMME

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

STAMP

Roughness evaluation

INJECTED PLASTIC

On substrate



Ra: 4.815 nm Sq: 6.3076 nm 860nm

On marks



2.4934 nm 3.9706 nm

Sq: Sq:









#### 4.- Next steps

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



PROGRAMME

### THANK YOU

#### TAK







