POLITECNICO DI MILANO

Stochastic Mechanical Characterization of Polysilicon MEMS: a Deep Learning Approach

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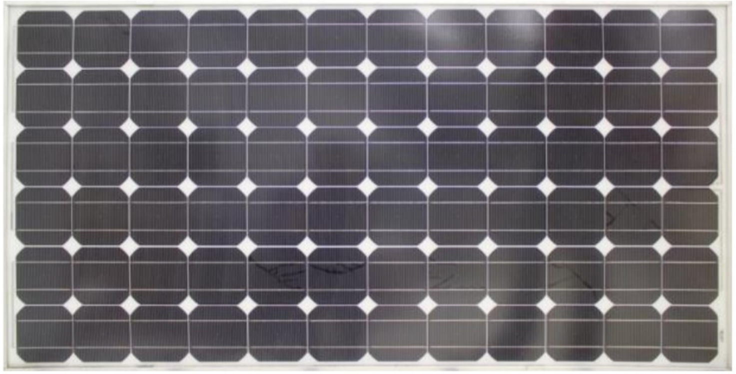
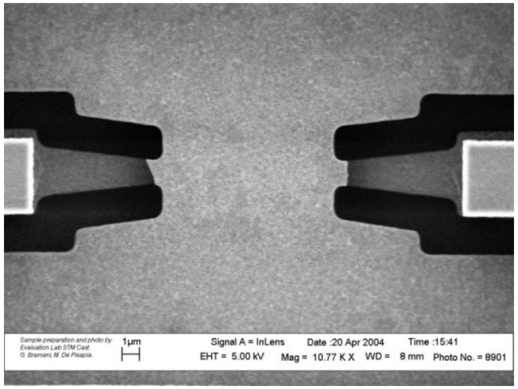
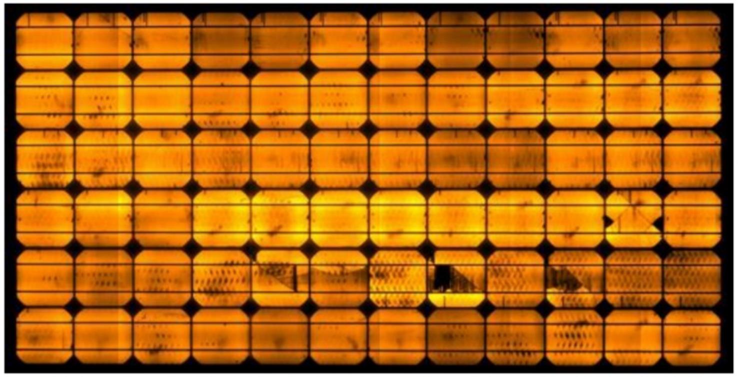
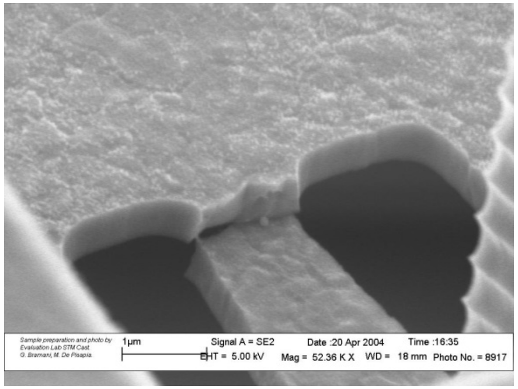
ENGINEERING MOTIVATION:
failure of POLYSILICON (thin) films exposed to mechanical and thermal loads

Due to mechanical and thermal loads, (thin) Si films can break because of the propagation of inter- and/or trans-granular cracks

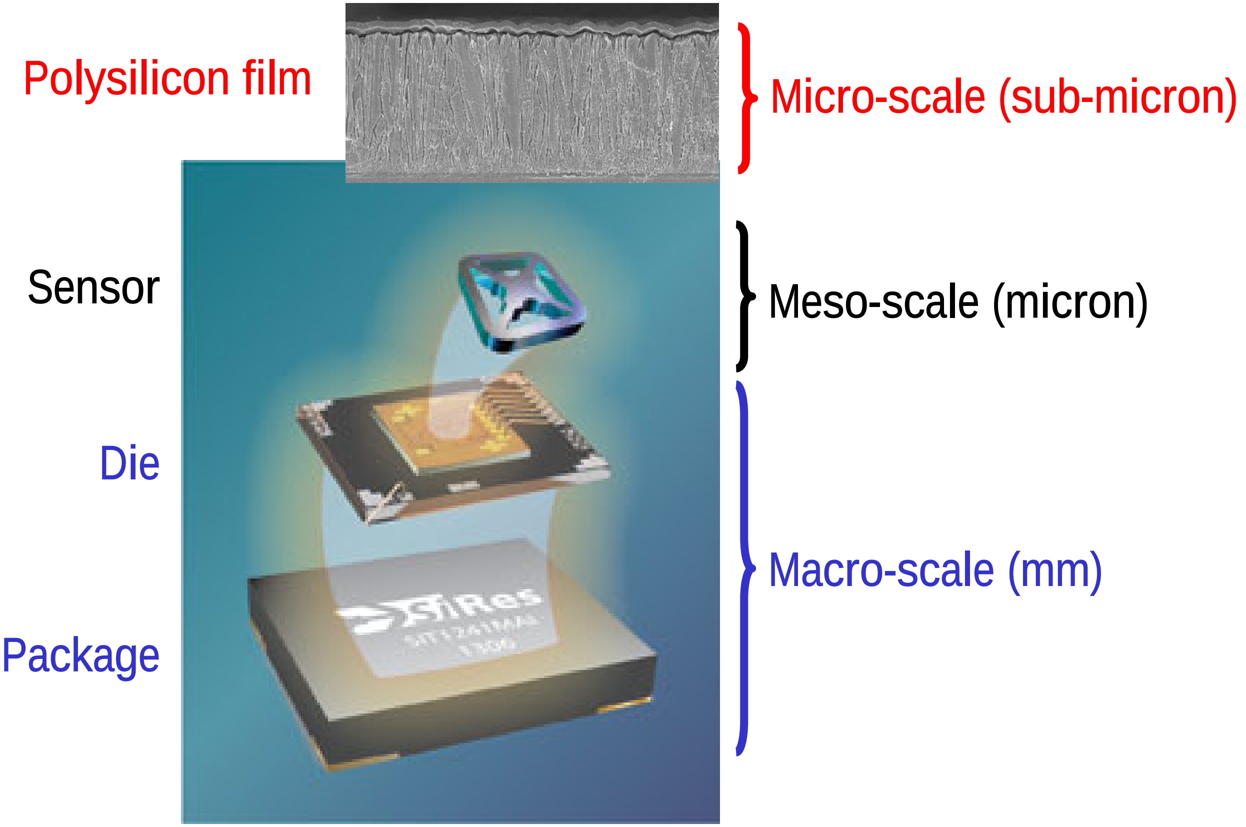








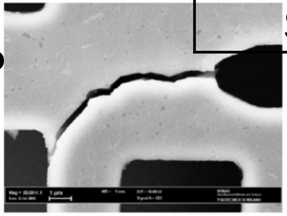
Length-scales in MEMS: from package to thin film mech.



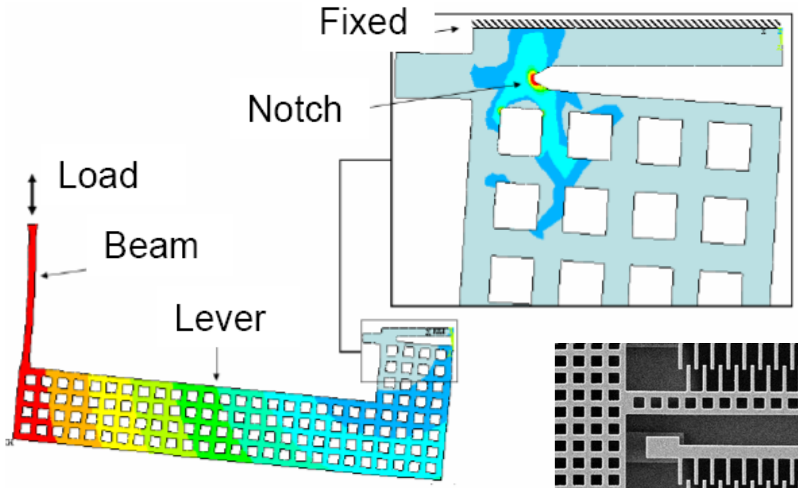
Multi-scale analysis of MEMS subject to mechanical shocks:

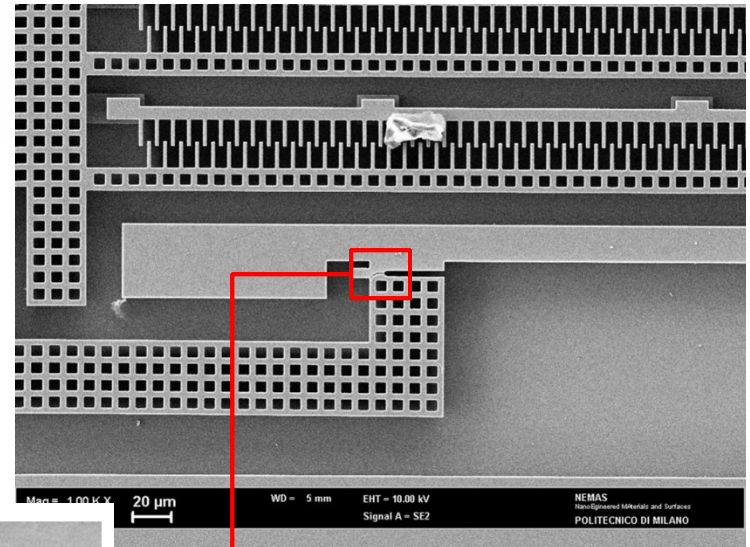
- decoupling between macro-scale and meso-scale allowed by small inertia of the sensor
- decoupling between meso-scale and micro-scale? (not allowed if nonlinear effects to be simulated)

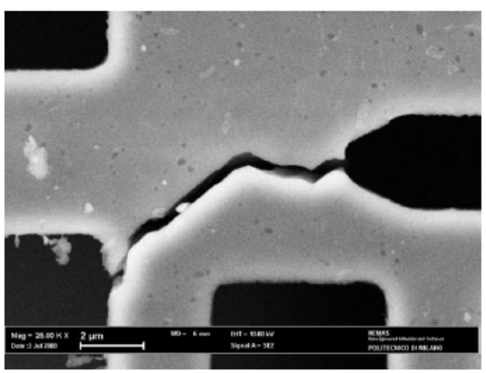
	mass (Kg)
Package	$5 \cdot 10^{-4}$
Die	$2.3 \cdot 10^{-6}$
Sensor	$3 \cdot 10^{-9}$

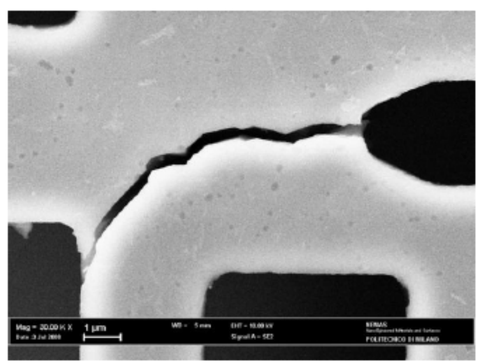


On-chip testing (crack and fatigue)









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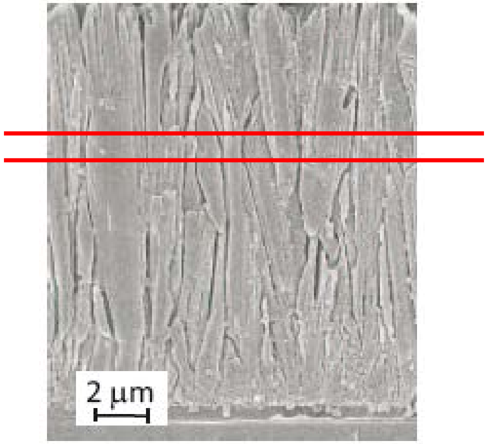
Meso-scale elastic properties

Micro-scale analysis: upscaling of elastic properties
Homogenization approach

Columnar polysilicon film
(lateral view)



taking a slice of the film
(plane stress cond.)

regularized Voronoi tessellations

Through homogenization: in-plane macro strain and stress components (vectors)

$$\boldsymbol{E} = \{E_{11} \quad E_{22} \quad E_{12}\}^{\mathrm{T}}$$
$$\boldsymbol{\Sigma} = \{\Sigma_{11} \quad \Sigma_{22} \quad \Sigma_{12}\}^{\mathrm{T}}$$

defined as volume averages, according to:

$$\boldsymbol{\Sigma} = \frac{1}{V}\int_V \boldsymbol{\sigma} dV$$

$$\boldsymbol{E} = \frac{1}{V}\int_V \boldsymbol{\varepsilon} dV$$

local elastic law

$$\boldsymbol{\sigma} = \boldsymbol{c}\boldsymbol{\varepsilon}$$

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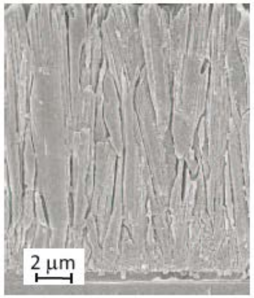
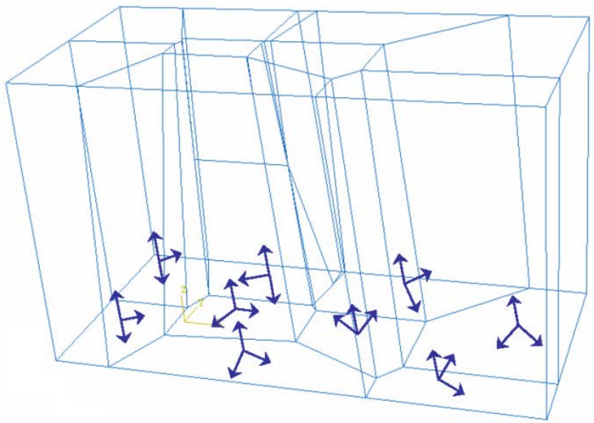
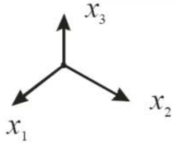
Polysilicon assumed to feature:

- one axis of elastic symmetry aligned with epitaxial growth direction x_3
- random orientation of other two elastic symmetry directions in the x_1- x_2 plane







Matrix of elastic moduli for single-crystal Si (FCC symmetry)

$$\mathbf{c} = \begin{bmatrix} 165.7 & 63.9 & 63.9 & 0 & 0 & 0 \\ 63.9 & 165.7 & 63.9 & 0 & 0 & 0 \\ 63.9 & 63.9 & 165.7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 79.6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 79.6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 79.6 \end{bmatrix} \quad GPa$$

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Micro-scale analysis: upscaling of elastic properties

Elastic moduli in $\boldsymbol{\Sigma} = \boldsymbol{C}\boldsymbol{E}$ are numerically bounded through:

- uniform strain boundary cond.

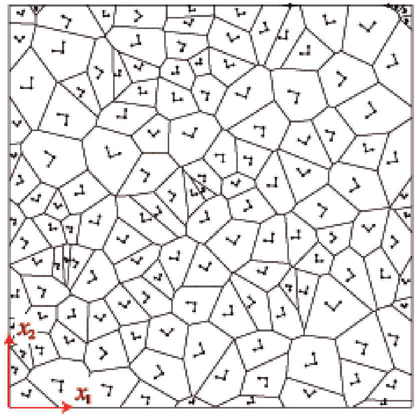
$$\boldsymbol{u} = \boldsymbol{X}\boldsymbol{E} \quad \text{on} \quad \partial V$$

- uniform stress boundary cond.

$$\boldsymbol{T} = \boldsymbol{N}\boldsymbol{\Sigma} \quad \text{on} \quad \partial V$$

$$\boldsymbol{X} = \begin{bmatrix} x_1 & 0 & \frac{x_2}{2} \\ 0 & x_2 & \frac{x_1}{2} \end{bmatrix}$$

$$\boldsymbol{N} = \begin{bmatrix} n_1 & 0 & n_2 \\ 0 & n_2 & n_1 \end{bmatrix}$$



Voigt and **Reuss** bounds:

from Hill-Mandel macro-homogeneity condition $\boldsymbol{\Sigma}^{\mathrm{T}}\boldsymbol{E} = \frac{1}{V}\int_V \boldsymbol{\sigma}^{\mathrm{T}}\boldsymbol{\varepsilon}\, dV = \frac{1}{V}\int_V \boldsymbol{\sigma}_l^{\mathrm{T}}\boldsymbol{\varepsilon}_l\, dV$

Voigt assumption: $\boldsymbol{\varepsilon} = \boldsymbol{E}$ everywhere

$$\boldsymbol{E}^{\mathrm{T}}\boldsymbol{C}\boldsymbol{E} = \frac{1}{V}\int_V \boldsymbol{\varepsilon}_l^{\mathrm{T}}\boldsymbol{c}_l\boldsymbol{\varepsilon}_l\, dV = \frac{1}{V}\int_V \boldsymbol{\varepsilon}^{\mathrm{T}}\boldsymbol{t}_\varepsilon^{\mathrm{T}}\boldsymbol{c}_l\boldsymbol{t}_\varepsilon\boldsymbol{\varepsilon}\, dV = \boldsymbol{E}^{\mathrm{T}}\left[\frac{1}{V}\int_V \boldsymbol{t}_\varepsilon^{\mathrm{T}}\boldsymbol{c}_l\boldsymbol{t}_\varepsilon\, dV\right]\boldsymbol{E} = \boldsymbol{E}^{\mathrm{T}}\left[\frac{1}{V}\int_V \boldsymbol{c}\, dV\right]\boldsymbol{E}$$

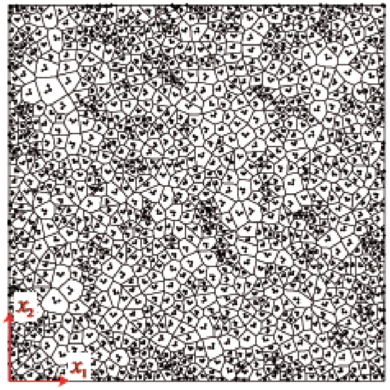
$$\Rightarrow \quad \boldsymbol{C} = \frac{1}{V}\int_V \boldsymbol{t}_\varepsilon^{\mathrm{T}}\boldsymbol{c}_l\boldsymbol{t}_\varepsilon\, dV$$

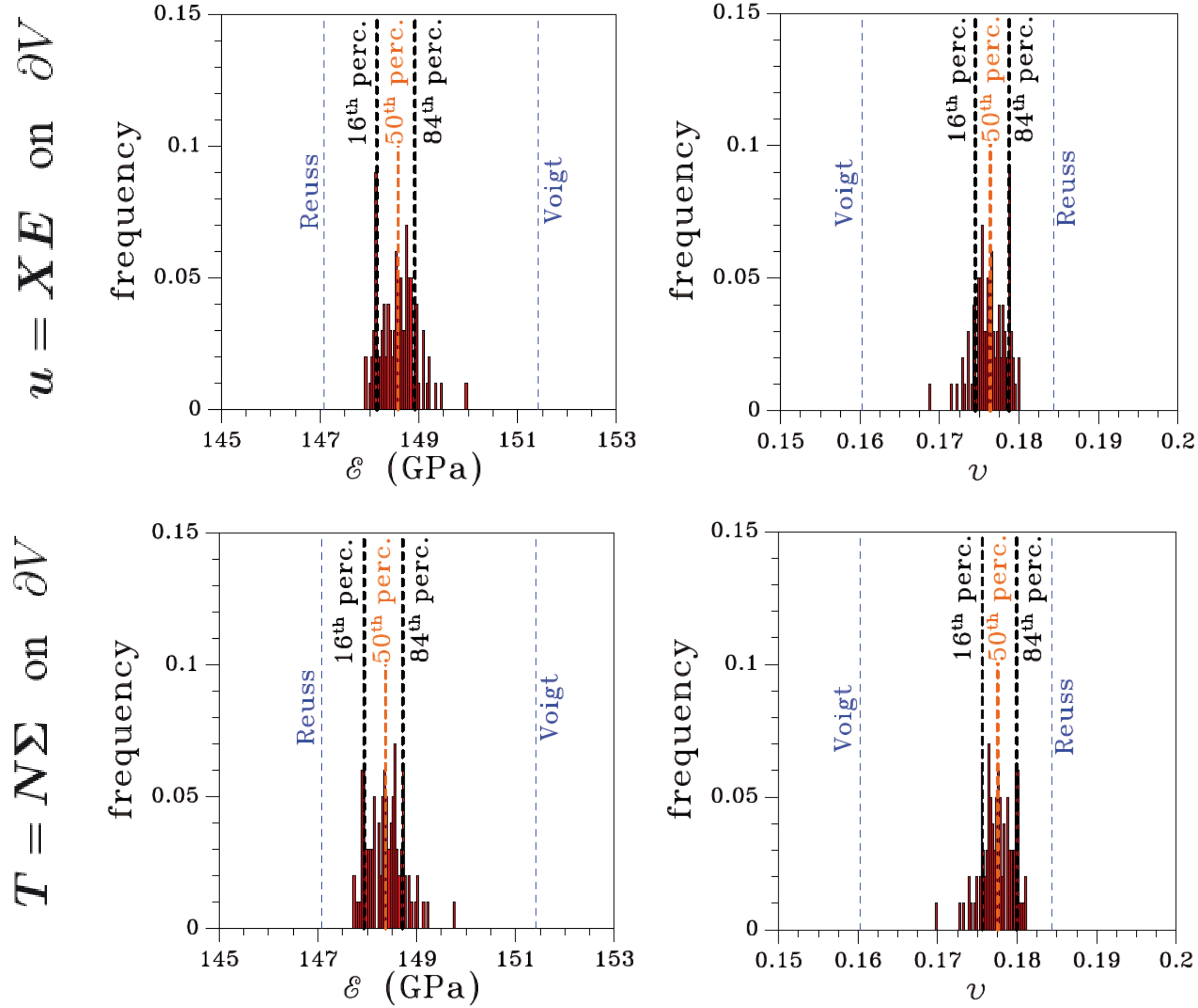
Reuss assumption: $\boldsymbol{\sigma} = \boldsymbol{\Sigma}$ everywhere

$$\Rightarrow \quad \boldsymbol{C}^{-1} = \frac{1}{V}\int_V \boldsymbol{t}_\sigma^{\mathrm{T}}\boldsymbol{c}_l^{-1}\boldsymbol{t}_\sigma\, dV$$

Micro-scale analysis: upscaling of elastic properties

$L = 12\ \mu m,$
$\bar{s}_g = 0.2\ \mu m$





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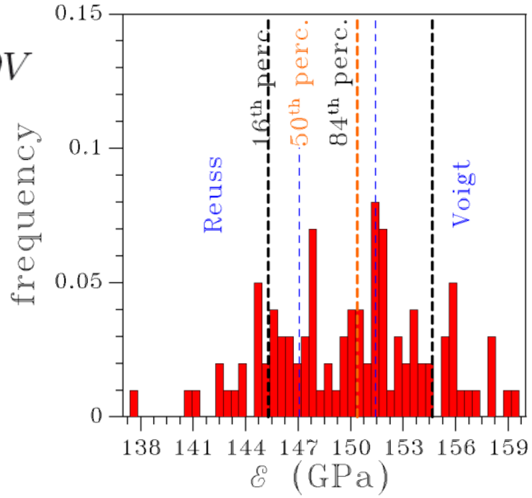
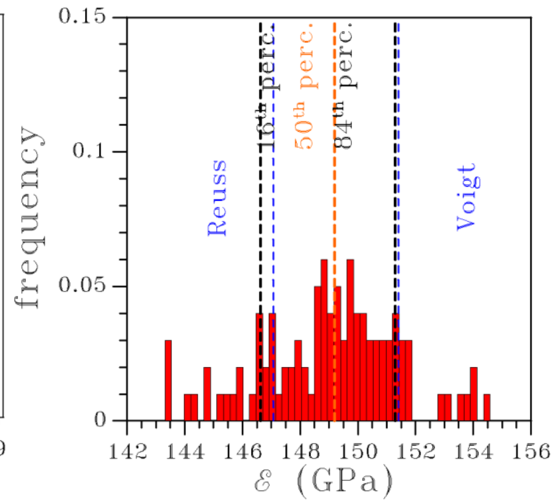
SVE size and upscaling of elastic properties

$\boldsymbol{u} = \boldsymbol{X}\boldsymbol{E} \quad \text{on} \quad \partial V$

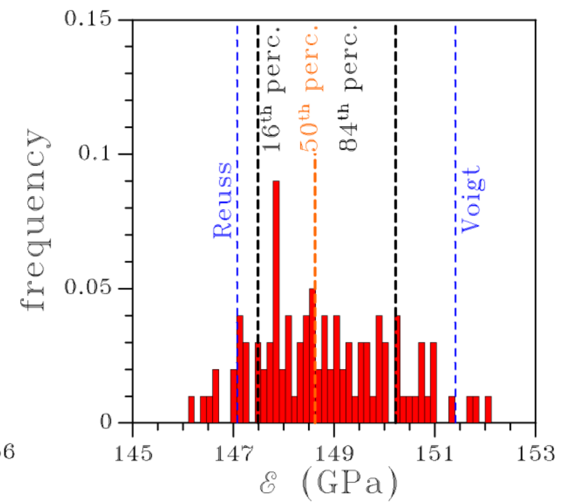
$\bar{s}_g = 0.6\ \mu\text{m}$



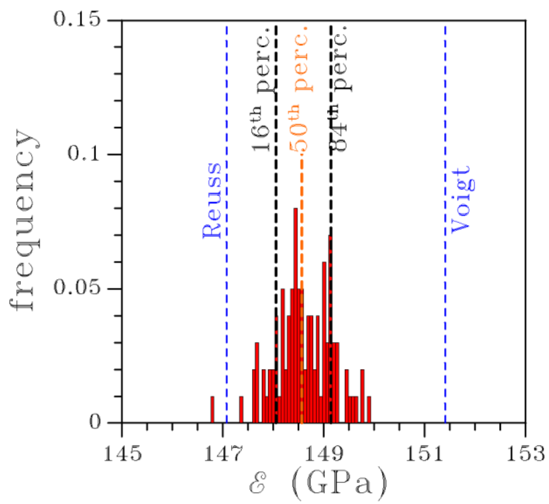
$L = 3\ \mu\text{m}$



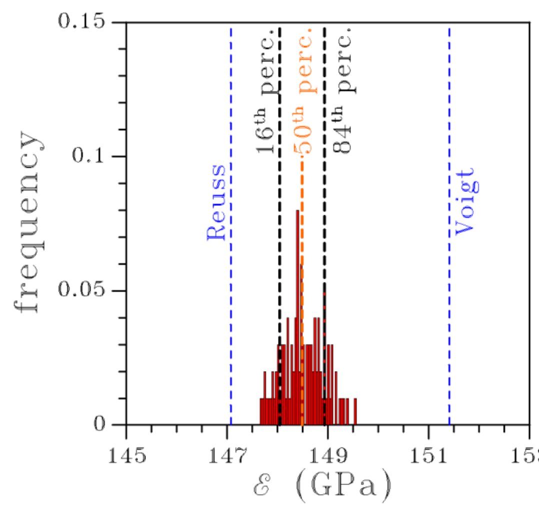
$L = 6\ \mu\text{m}$



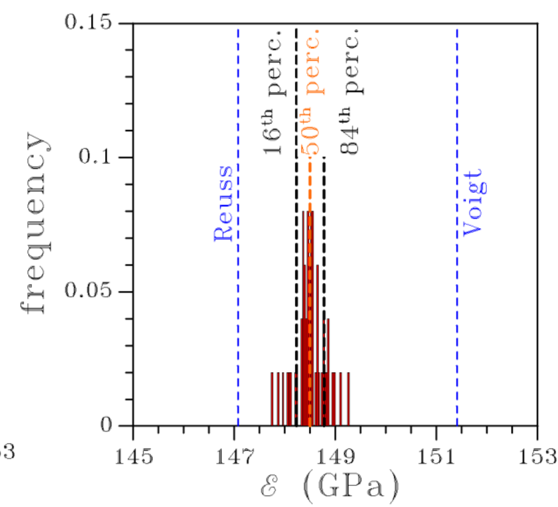
$L = 12\ \mu\text{m}$



$L = 24\ \mu\text{m}$



$L = 36\ \mu\text{m}$



$L = 48\ \mu\text{m}$

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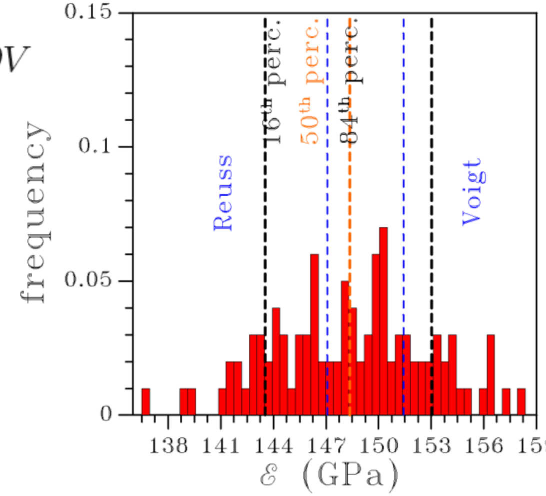
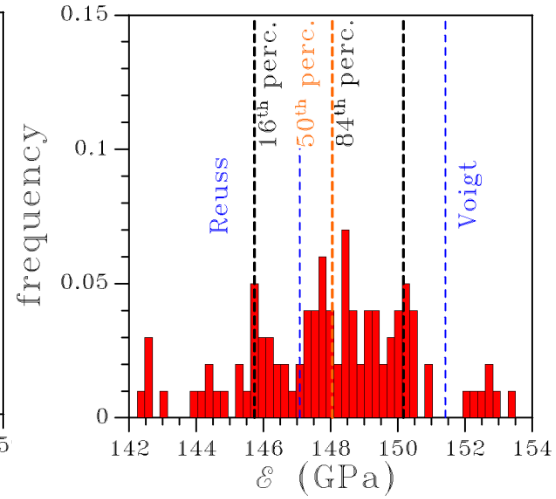
SVE size and upscaling of elastic properties

$\boldsymbol{T} = \boldsymbol{N\Sigma}$ on ∂V

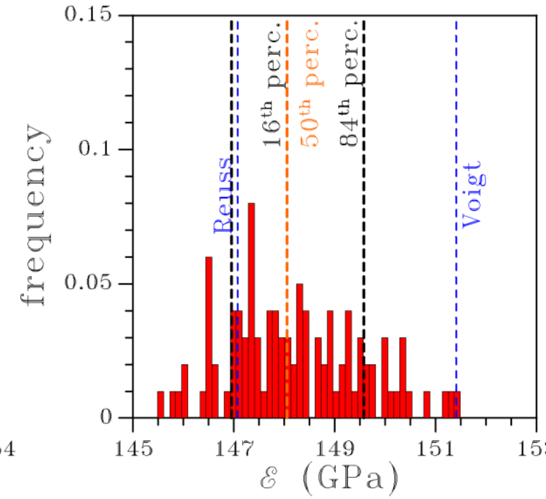
$\bar{s}_g = 0.6\ \mu\text{m}$



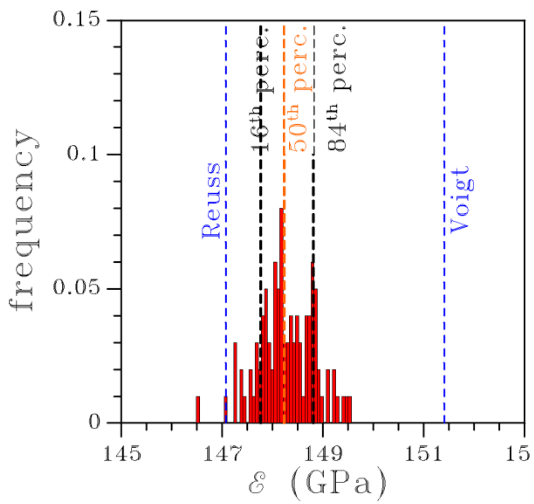
$L = 3\ \mu\text{m}$



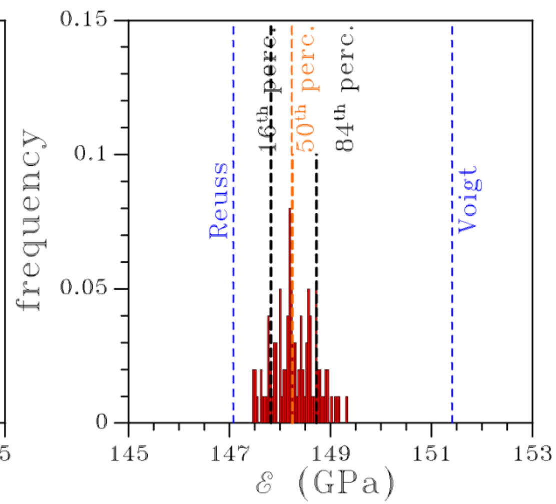
$L = 6\ \mu\text{m}$



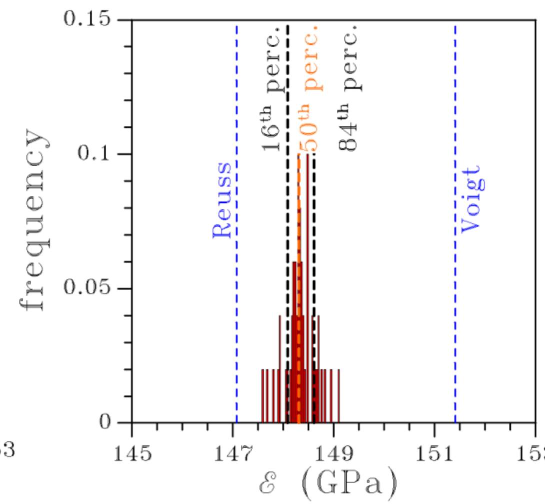
$L = 12\ \mu\text{m}$



$L = 24\ \mu\text{m}$



$L = 36\ \mu\text{m}$



$L = 48\ \mu\text{m}$

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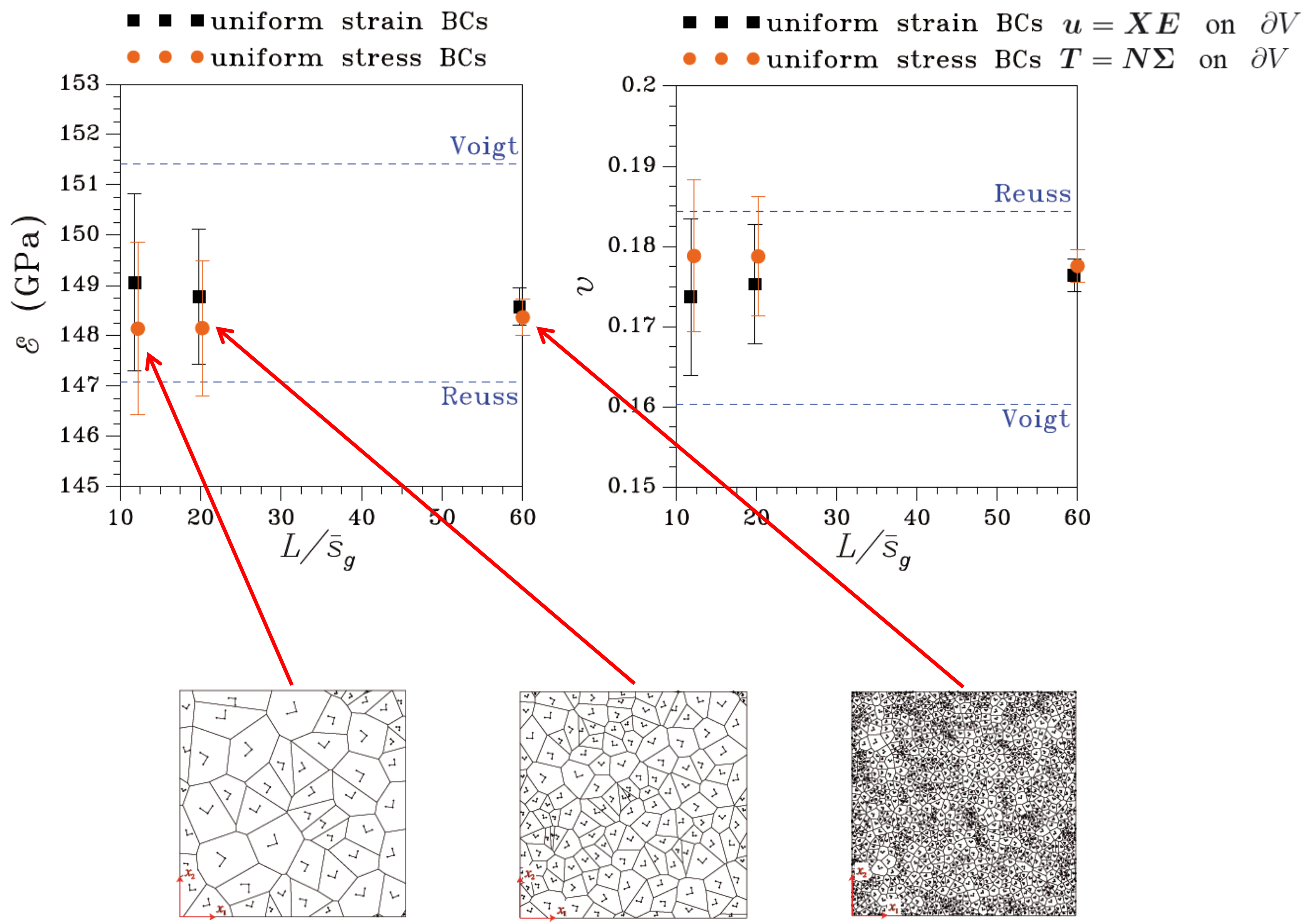
Micro-scale analysis: upscaling of elastic properties



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Micro-scale analysis: upscaling of elastic properties
Deep Learning approach

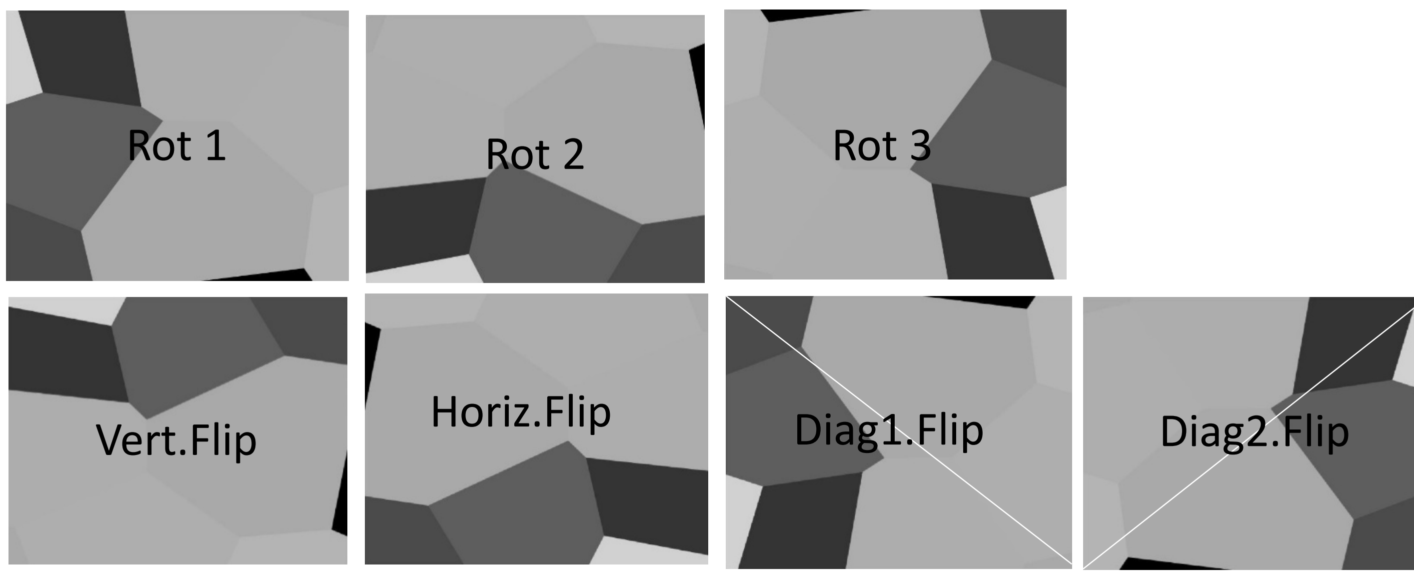
INPUT DATA

Images resolution= 256x256

Color scale indicate
rotations 0°- 45°

192 SVE images+ data augmentation > 1536 images
(1152 images for training and 384 images for validation)

Data augmentation



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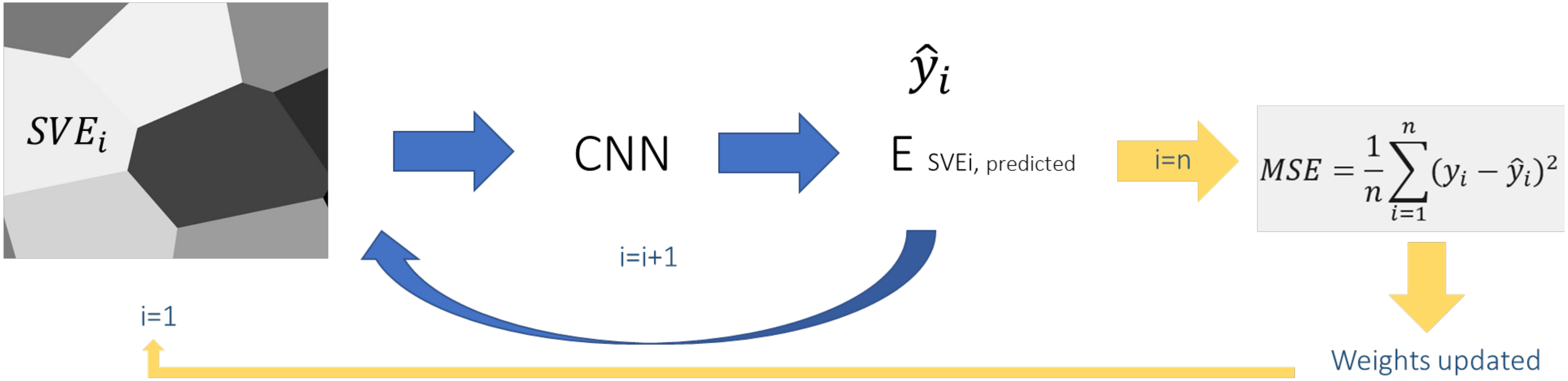
SOME RELEVANT HYPERPARAMETERS

- Optimizer=Adam(lr=5e-4, decay=5e-4/200)
- Loss Function=Mean Squared Error
- Training epochs=100
- Batch size = 32

TRAINING PROCEDURE

Scheme for 1 epoch



Convolutional Neural Network (CNN) and Deep Learning

SVE´s VALIDATION SET → Trained CNN → Effective Young´s modulus prediction

↓

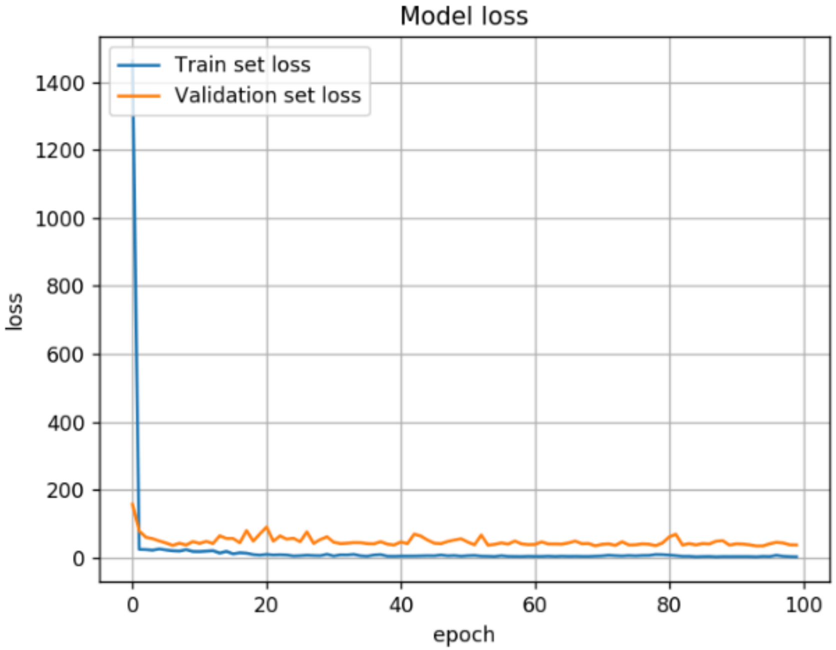
FINAL ASSESSMENT

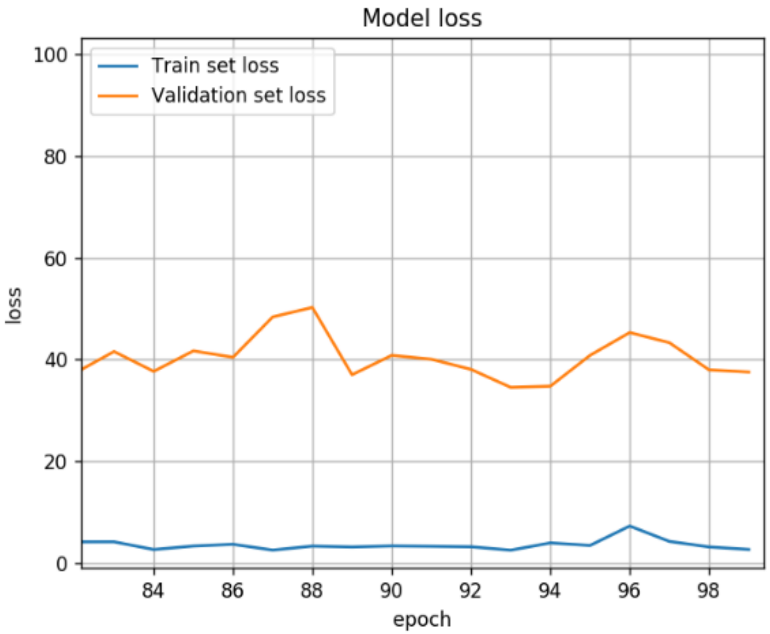
Mean of the predictions
Standard deviation of the predictions

vs

Mean of the labeled data
Standard deviation of the labeled data

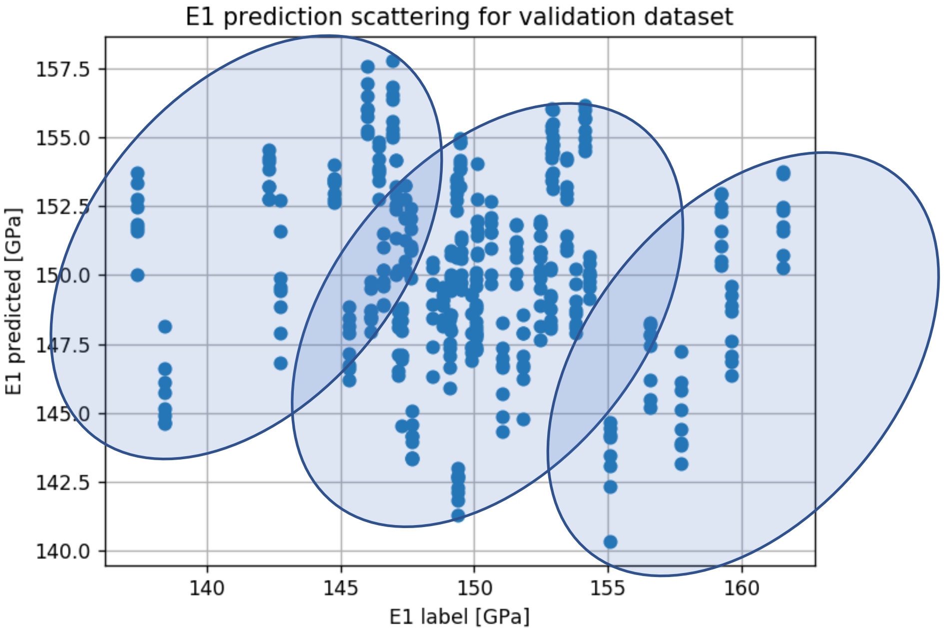
CNN training and validation

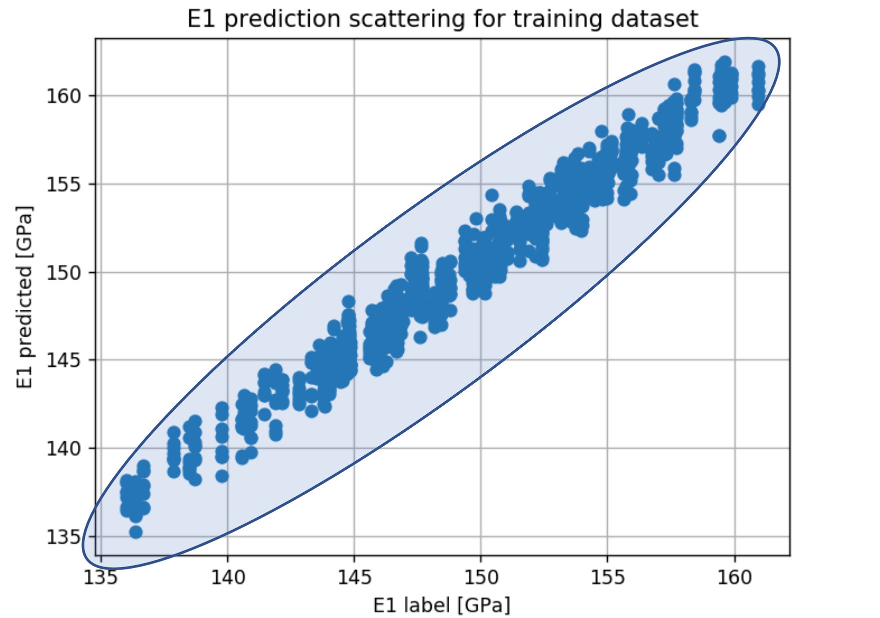




Final training loss = 2.6787 GPa^2
Final validation loss = 37.5667 GPa^2

CNN predictions





E_m = 150.0 GPa, E_s = 3.4 GPa for the validation set

vs

E_m = 149.9 GPa, E_s = 4.8 GPa
for the validation set labels

0,067% absolute error in E1 Mean
29,16% absolute error in E1 Standard Deviation

E_m = 150.5 GPa, E_s = 5.5 GPa for the training set.

vs

E_m = 149.7 GPa, E_s = 5.5 GPa
for the labeled training set labels

0,53% absolute error in E1 Mean
0% absolute error in E1 Standard Deviation

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