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Homogénéisation numérique du comportement de matériaux hétérogènes

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1 – Homogénéisation numérique

1.1 : Principes

1.2 : Procédures CAST3M

2 – Applications

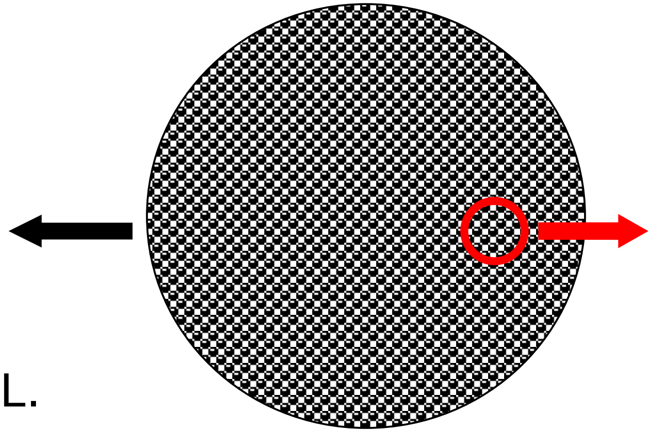
2.1 : Effet de la macro-porosité sur le comportement élastique des composites SiC/SiC

2.2 : Effets des joints de grains sur la conductivité thermique des polycristaux de SiC

Homogénéisation numérique : principes

Volume Elémentaire Représentatif

Volume Elémentaire Statistique



Comportement Effectif

Comportement Apparent

Insensible au choix des C.L.

Sensible au choix des C.L.

Moyenne statistique

Grosses « machines »!

Estimations du comportement Effectif (Petites « machines »!)

Homogénéisation numérique : principes

Propriétés en élasticité

$\overline{K_{CL}^{app}}$ Moyenne statistique sur un grand nombre de VES

$\overline{K_{P}^{app}}$ est une estimation de K^{eff}

$\overline{K_{DH}^{app}}$ est une borne supérieure de K^{eff}

$\left(\overline{(K_{CH}^{app})^{-1}}\right)^{-1}$ est une borne inférieure de K^{eff}

taille des VES $\nearrow$ ⇒ Écart entre les bornes $\searrow$
Vitesse de convergence statistique $\nearrow$
Durée de chaque calcul $\nearrow$

⇒ Compromis temps/précision

Homogénéisation numérique : procédures CAST3M

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- Application de conditions aux limites

RIGCL0 DEPI0 = NOMPROC MAIL0 TAB1;
* TAB1 = tenseur imposé
* Utilisation : DEP0 = RESOU (RIGMAT0 ET RIGCL0) DEPI0;

<u>MECANIQUE</u>

CLPD	Périodique	Déformation imposée
CLPC	Périodique	Contrainte imposée
CLCH	Contrainte homogène	Contrainte imposée
CLDH	Déformation homogène	Déformation imposée
CLDHC	Déformation homogène	Contrainte imposée
CLMI1	Mixte 1	Contrainte imposée
CLMI2	Mixte 2	Contrainte imposée

<u>THERMIQUE</u>

CLTH	Gradient de T homogène	Gradient de T
CLPT	Périodique	Gradient de T
CLFH	Flux homogène	Flux

- Evaluation du comportement apparent

KAPP0 CONT0 DEF0 = KEFF MOD0 MAT0 NOMPROC0 AMPL0 CONV0 VISU0;
KEFFT

Homogénéisation numérique : Applications

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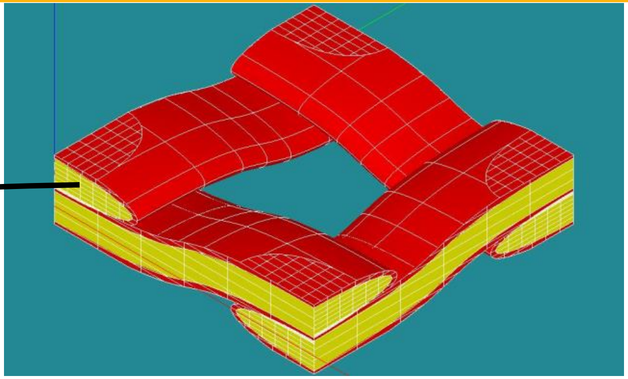
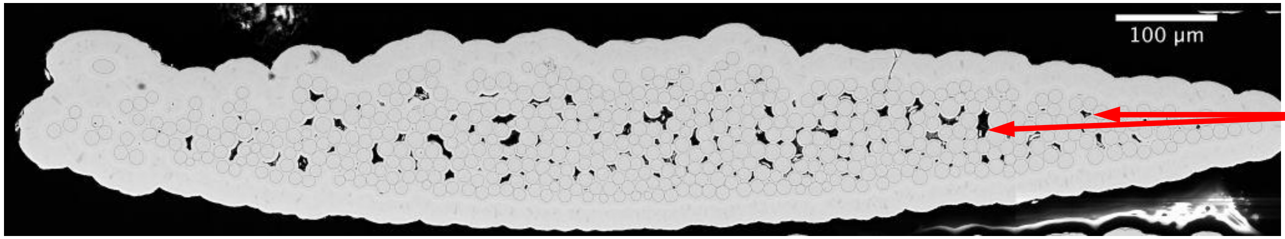
- ✓ 2D plain weave architecture
- ✓ 13 plies
- ✓ Fibres : Hi-Nicalon S (~13µm)
- ✓ Matrix : CVI



3D geometrical modelling of the plain weave pattern

SEM section of a tow:

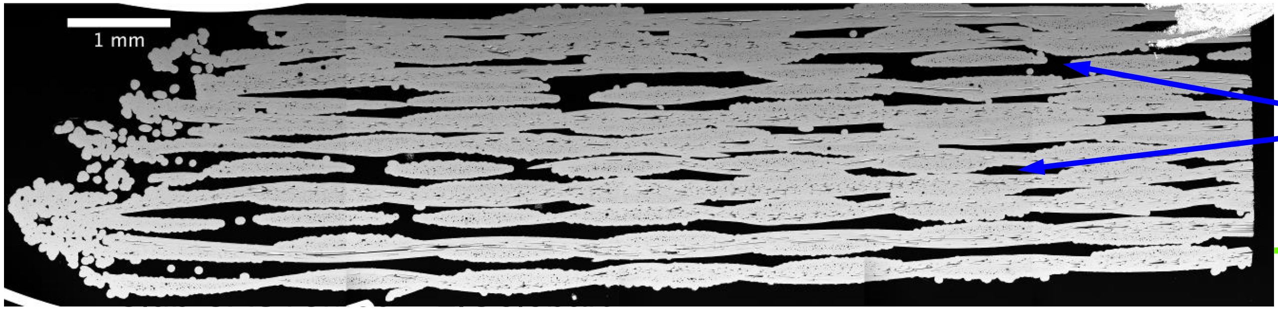
0.1mm



mIcro-porosity ~5%
Fibres (500,~55%)
(=> JNM, 2009
+ PhD thesis C. Château,)

SEM section of the whole composite

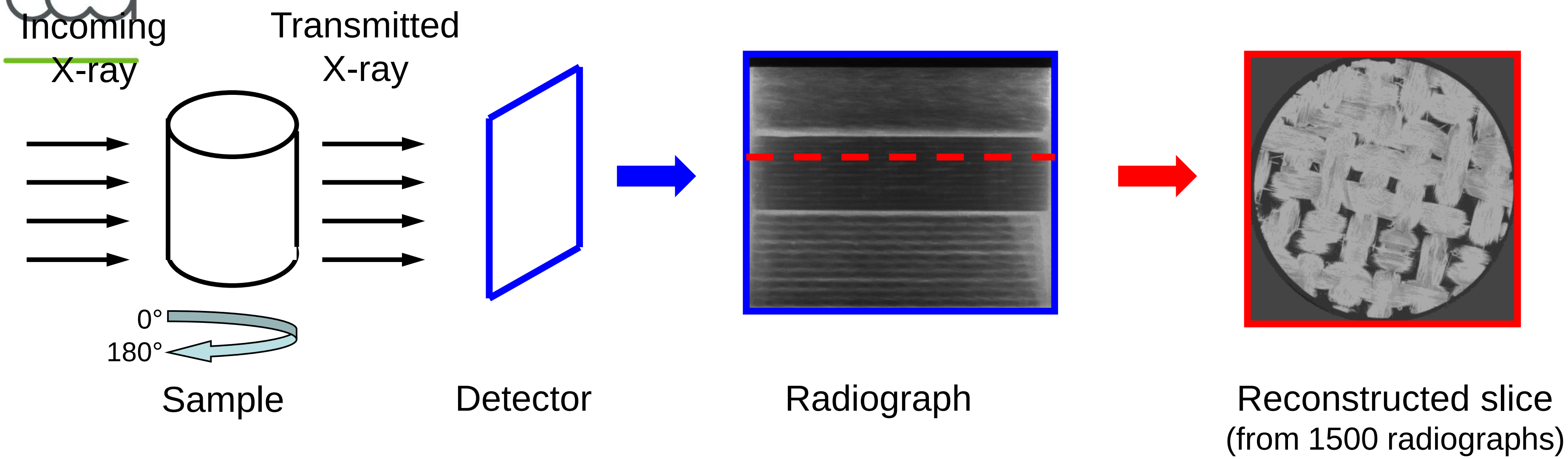
1mm



mAcro-porosity
3D open porosity
very complex shape

Homogénéisation numérique : Applications

➢ Principle of X-ray tomography



➢ Main characteristics of X-ray tomograhy on the ID19 beamline (ESRF)

Resolution (« voxel » size) :	$5.02^3 \mu m^3$
Field of view :	10.28mm (diameter) x 8.53mm (height)

Observation of the macro-porosity on a representative volume element

Homogénéisation numérique : Applications

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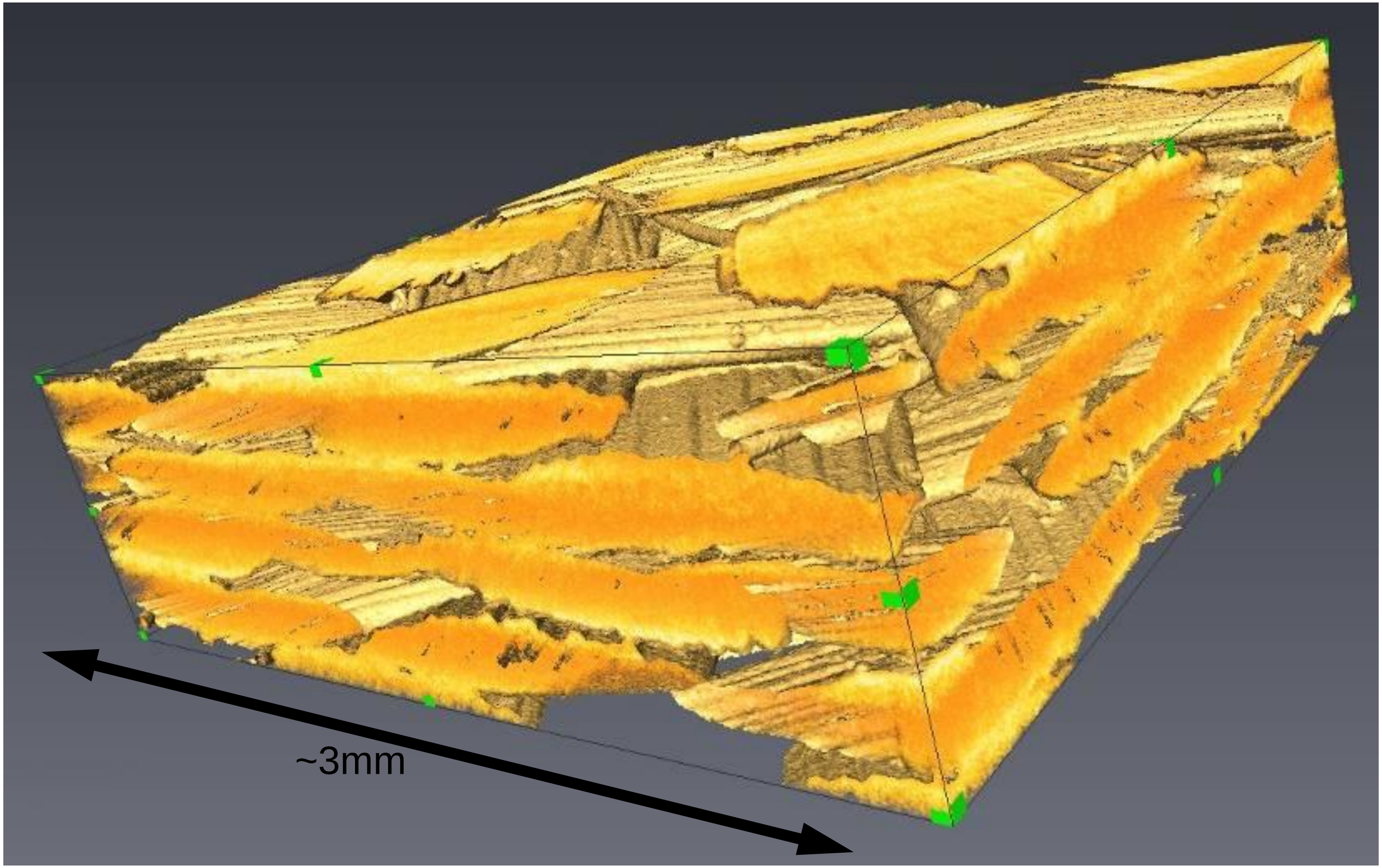

A 3D visualization of the microstructure

Homogénéisation numérique : Applications

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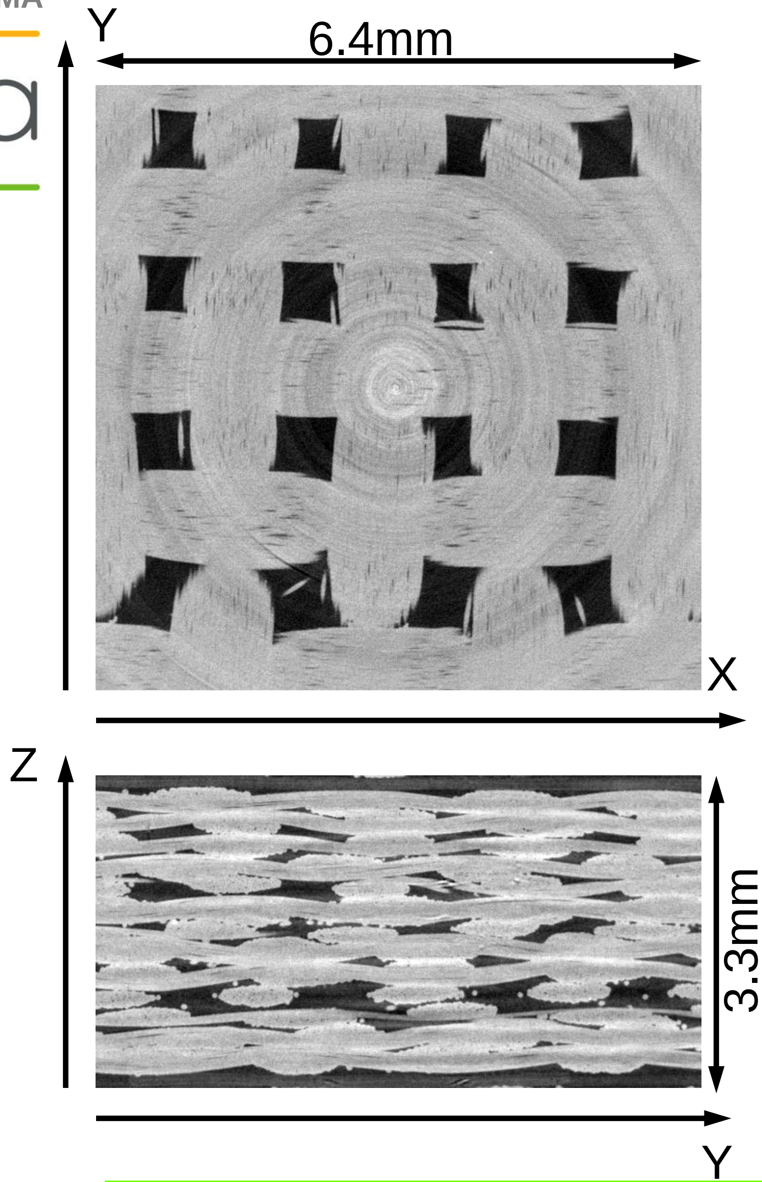
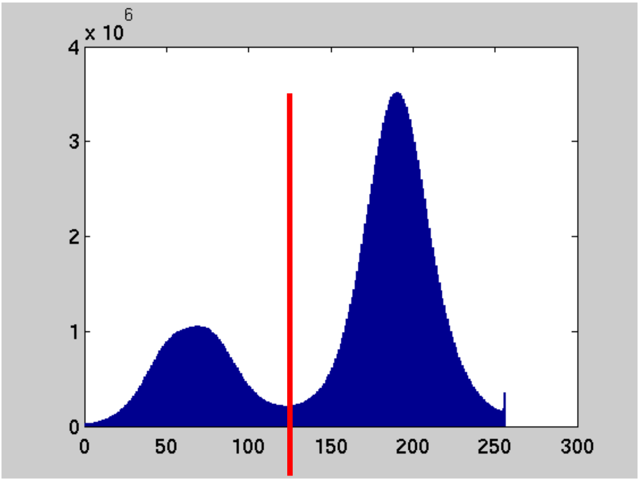
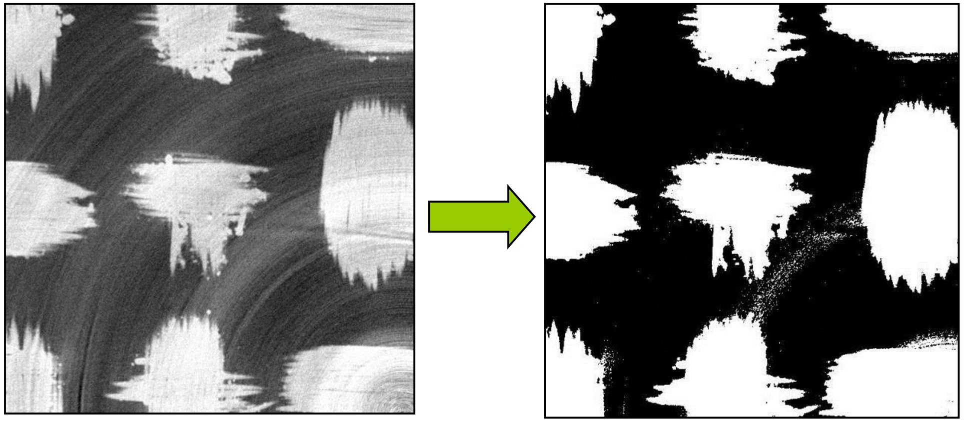
- Region of interest
- Threshold operation







$F_{por} = 26,5\%$

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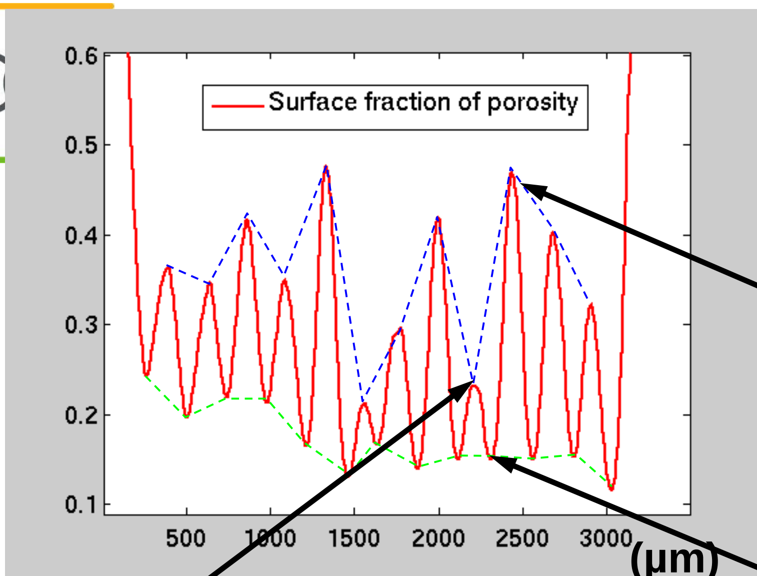
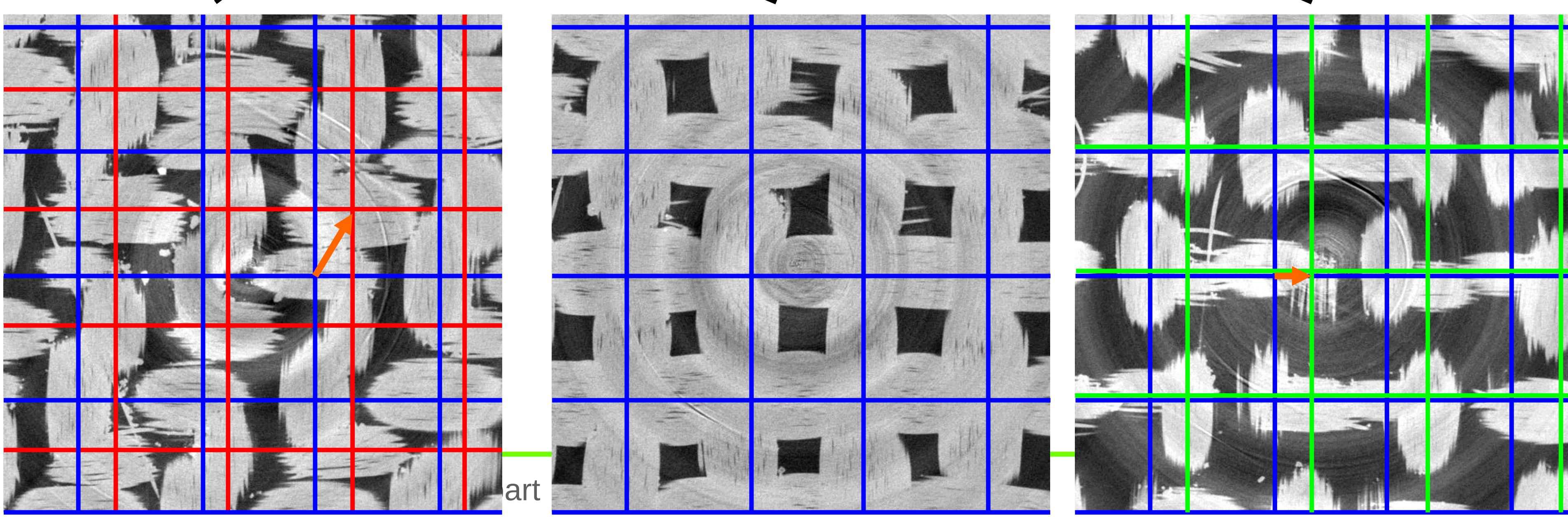
Homogénéisation numérique : Applications

➢ Evolution of the surface fraction of porosity in the Z-direction



Minimum = median plane within a ply

Maximum = median plane between two plies



Homogénéisation numérique : Applications

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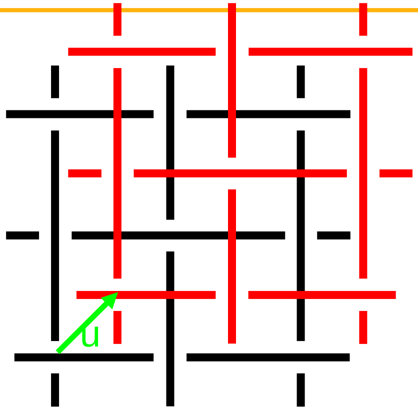
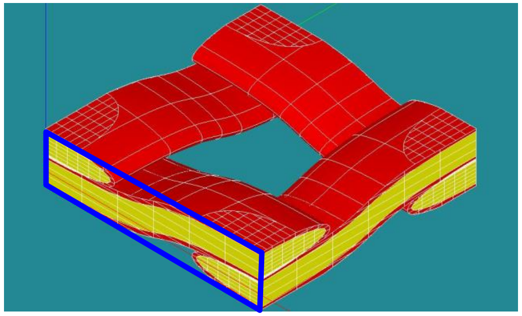
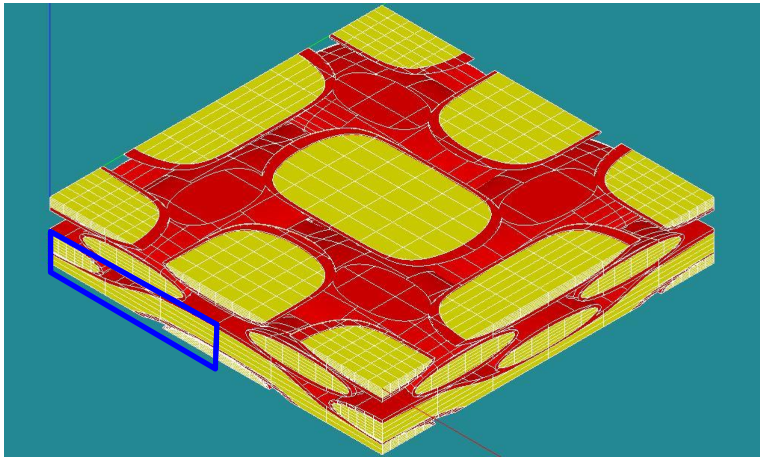
- Discussion with a geometrical model





Periodic unit-cell = one ply

Fporosity = 41%



Periodic unit-cell = two plies

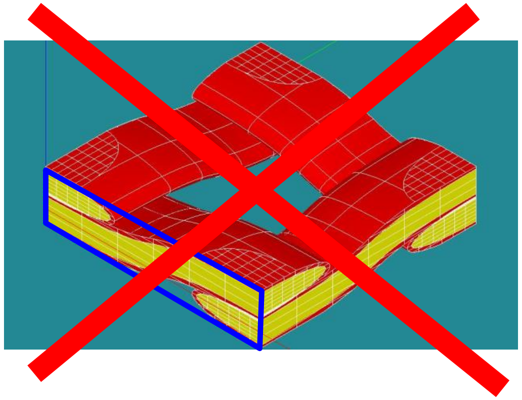
Fporosity = 21%

Volume fraction of porosity strongly depends on the stacking of the plies

Homogénéisation numérique : Applications

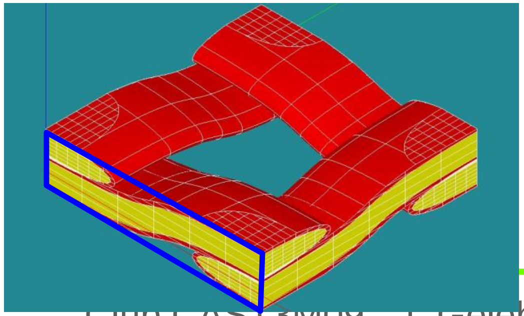
➢ Consequences on the micro-mechanical modelling

❑ Only one Volume Element (or unit-cell) with only one ply is not sufficient



❑ To account for the variability of the stacking of the plies :

- several volume elements (« Statistical Volume Elements »)
- at least two plies per volume element



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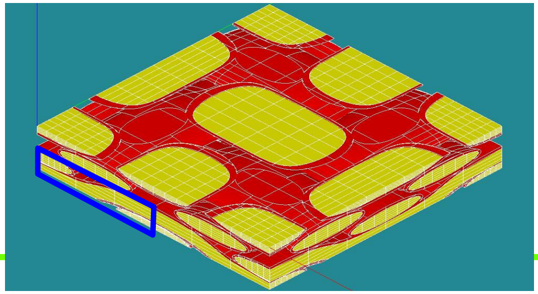

+ . . .

Homogénéisation numérique : Applications

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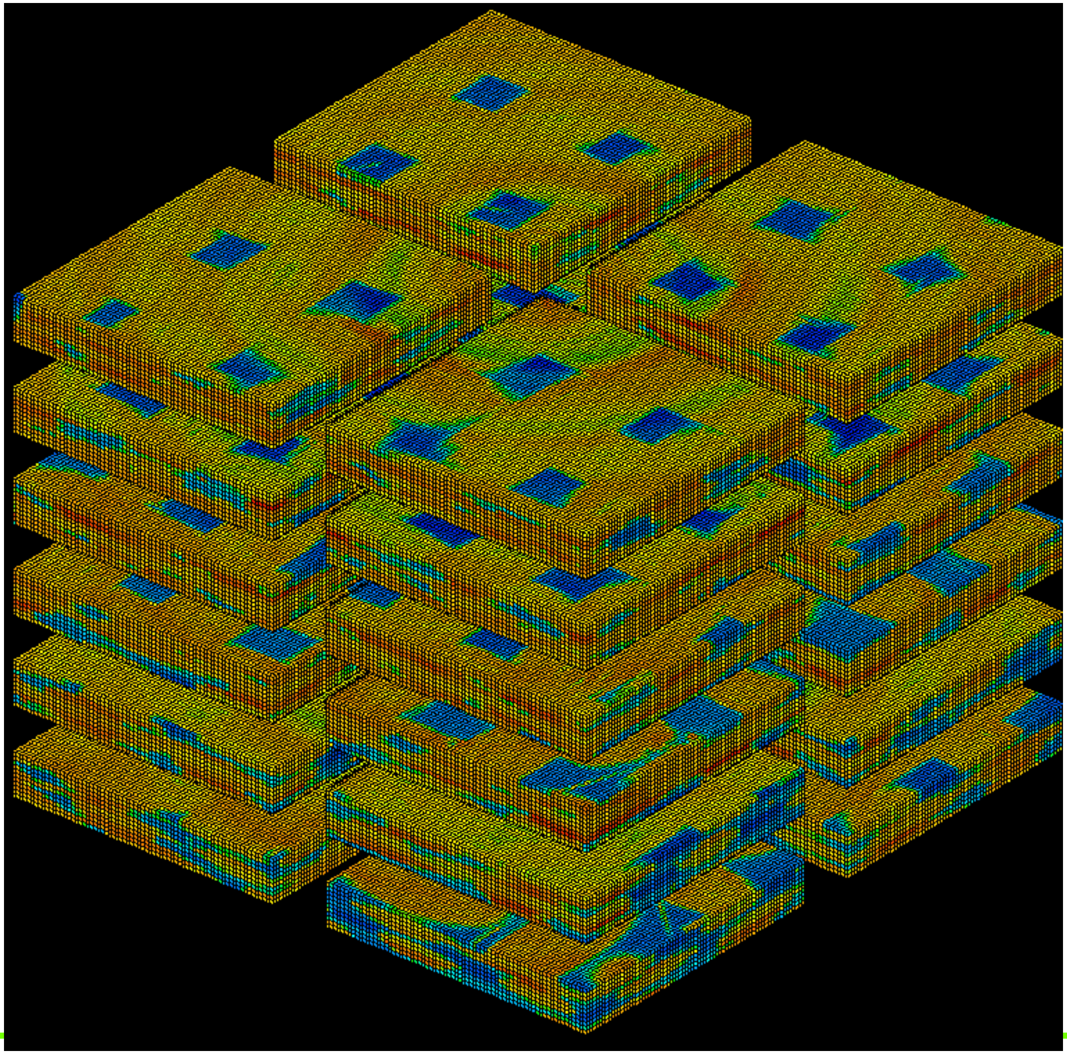
➢ Definition of the « Statistical Volume Elements »

24 SVE directly extracted from the tomographic image



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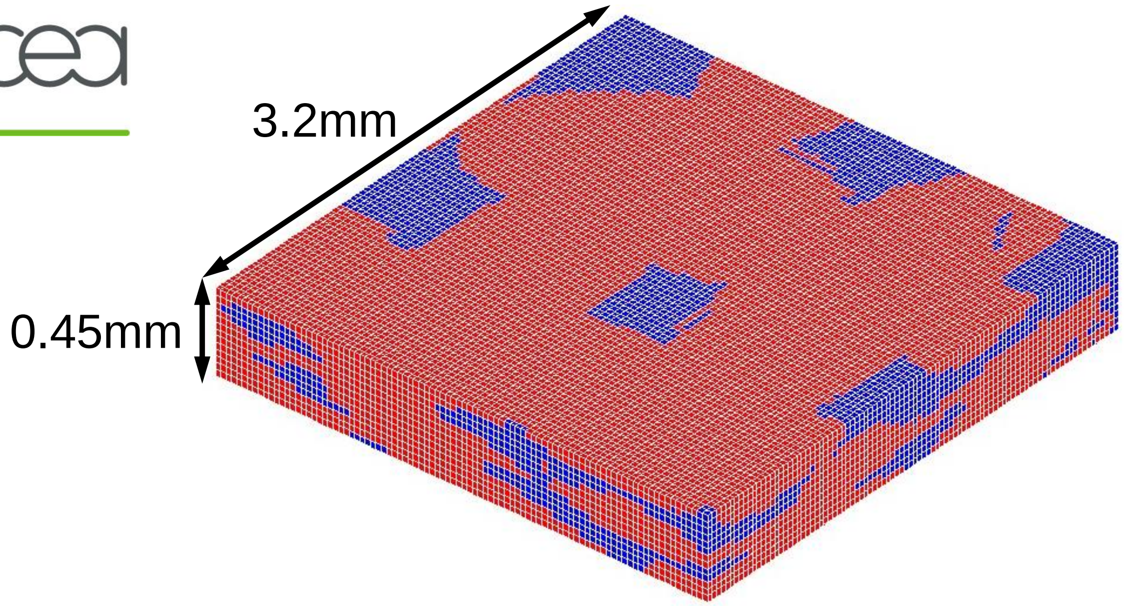
Homogénéisation numérique : Applications

➢ Definition of the « Statistical Volume Elements »



(110000elements)

<u>Material properties</u>

Composite

E = 400GPa,

nu = 0.3

Porosity

E =0.0004GPa

nu=0,3

Homogénéisation numérique : Applications

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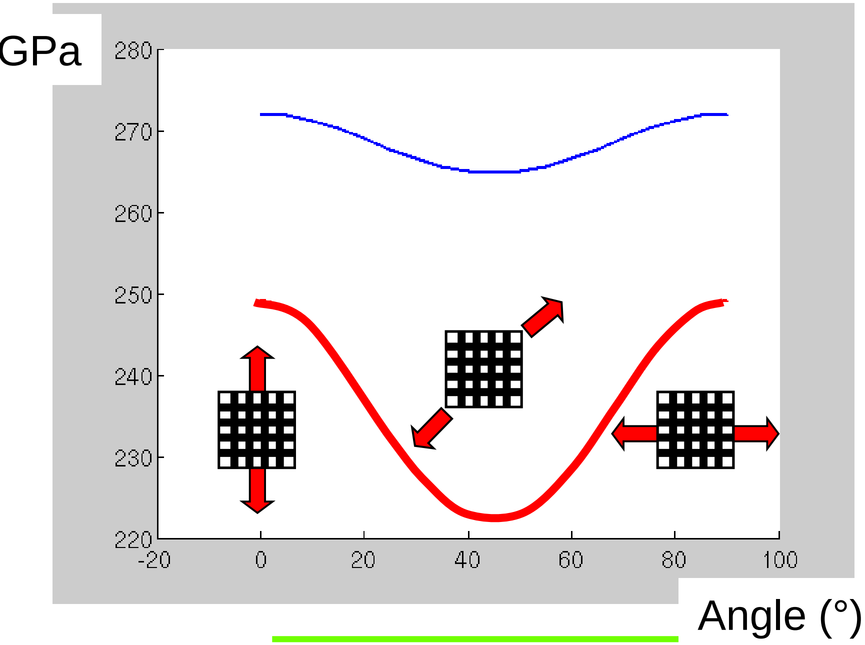
- Results : anisotropy of the « effective » behaviour

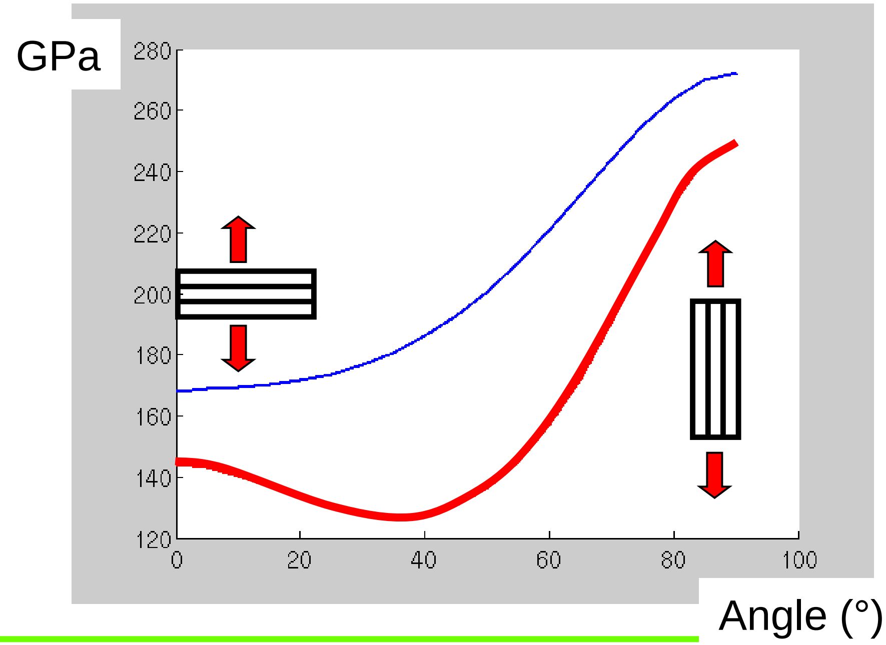
$$K_{PBC}^{eff} = \begin{pmatrix} 289 & 83 & 58 & 1 & 2 & 0 \\ & 278 & 53 & 1 & 1 & 0 \\ & & 161 & 0 & 1 & 0 \\ & & & 84 & 0 & 0 \\ & SYM & & & 52 & 0 \\ & & & & & 39 \end{pmatrix} \rightarrow \begin{pmatrix} 284 & 83 & 56 & 0 & 0 & 0 \\ & 284 & 56 & 0 & 0 & 0 \\ & & 161 & 0 & 0 & 0 \\ & & & 84 & 0 & 0 \\ & SYM & & & 46 & 0 \\ & & & & & 46 \end{pmatrix}$$

Exact quadratic symetry

Young modulus in the (X-Y)plane



Young modulus in the (X-Z)plane

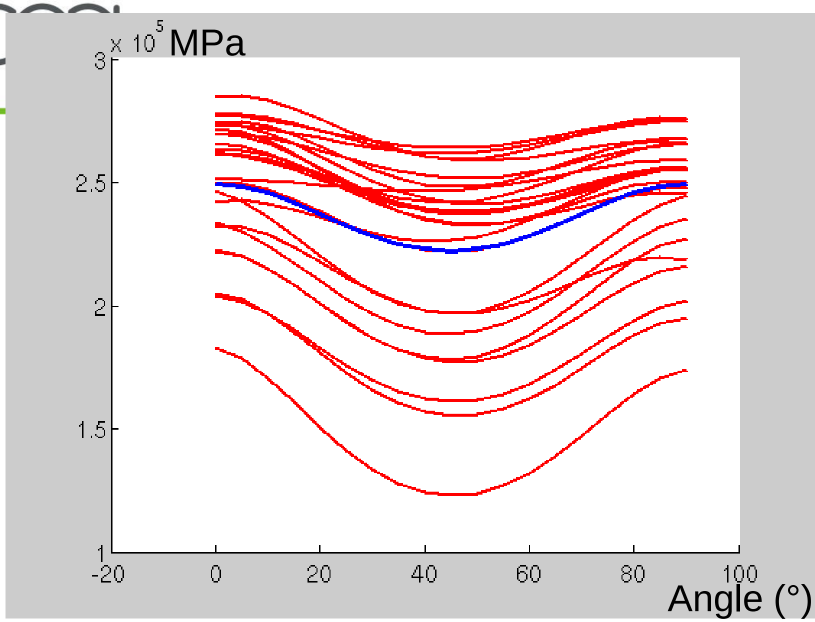


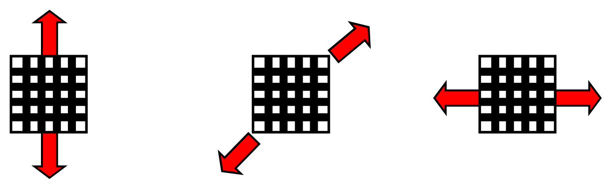
Red = periodic estimation, Blue = upper bound (KUBC)

Homogénéisation numérique : Applications

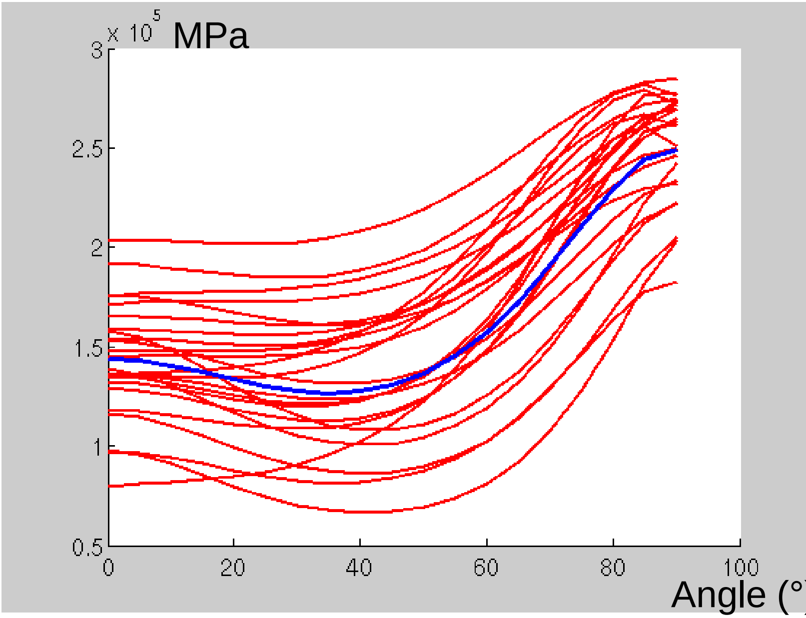
➢ Results : fluctuations of the « apparent » behaviours

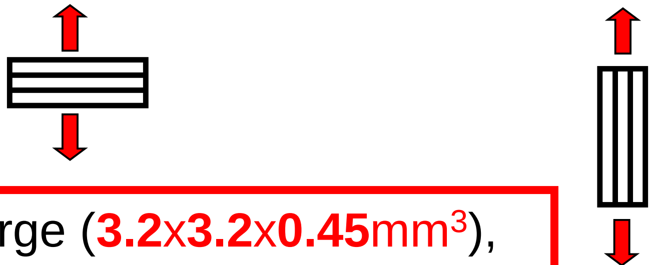
Young modulus in the (X-Y)plane





Young modulus in the (X-Z)plane





Even if the size of the volume element is quite large (**3.2**x**3.2**x**0.45**mm^3), important fluctuations are observed on the "apparent" behaviour

« Open » question : how to take into account this variability in the calculations of a SiC/SiC component?

Homogénéisation numérique : Applications

CONCLUSIONS

2D SiC/SiC composites have been characterized by X-ray tomography
the variability of the stacking of the plies strongly influences the porosity distribution

To account for this variability in micro-mechanical modeling
- several volume elements (« Statistical Volume Element » (SVE))
- at least two plies per volume elements

The effect of the macroporosity has been evaluated on the the «elastic » behaviour:
- the macroprorosity induces an anisotropic « effective » behaviour
- the macroporosity induces important fluctuations, even for a quite important size of the volume element (3.2x3.2x0.45mm3),

FUTURE PROSPECTS

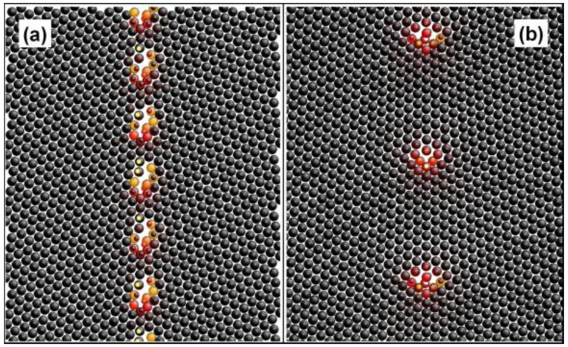
Thermal behaviour (on-going calculations, very similar results)
Introduction of the anisotropy of the tow (due to the micro-porosity)

Homogénéisation numérique : Applications

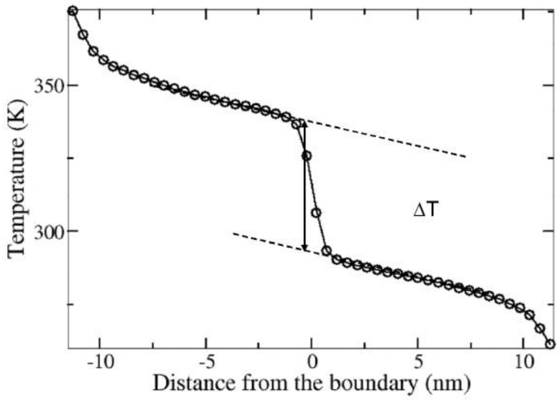
Effect of grain boundaries on the thermal conductivity of SiC polycrystals from discrete to continuous modeling

***Jour. Applied Physics**, Crocombette J.P., Gélébart L., 106, 083520 (2009)*

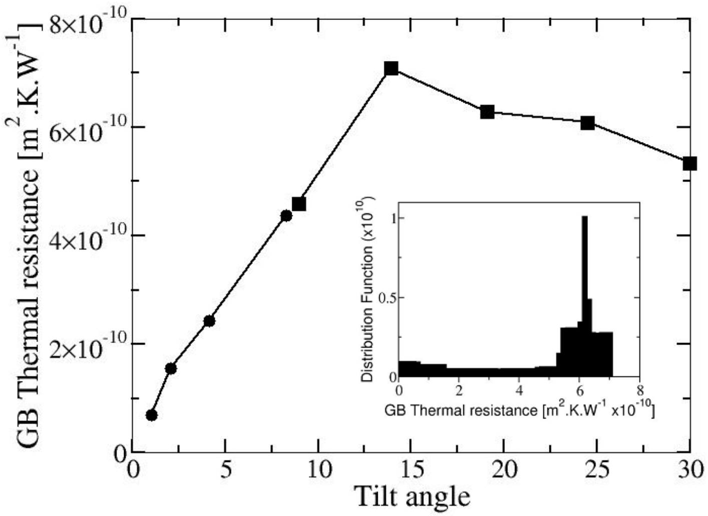
Grain boundary definition



Thermal calculation



$$q = -h\Delta T$$



Homogénéisation numérique : Applications

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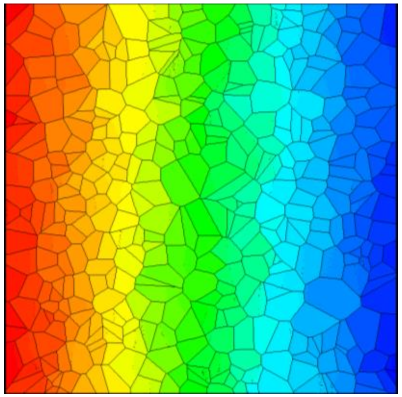
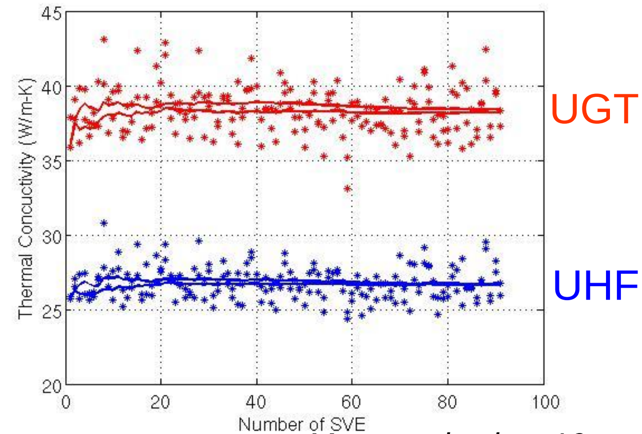
Finite Element simulation
UGT or UHF boundary conditions

Heterogenities :
- Grain sizes
- GB resistances

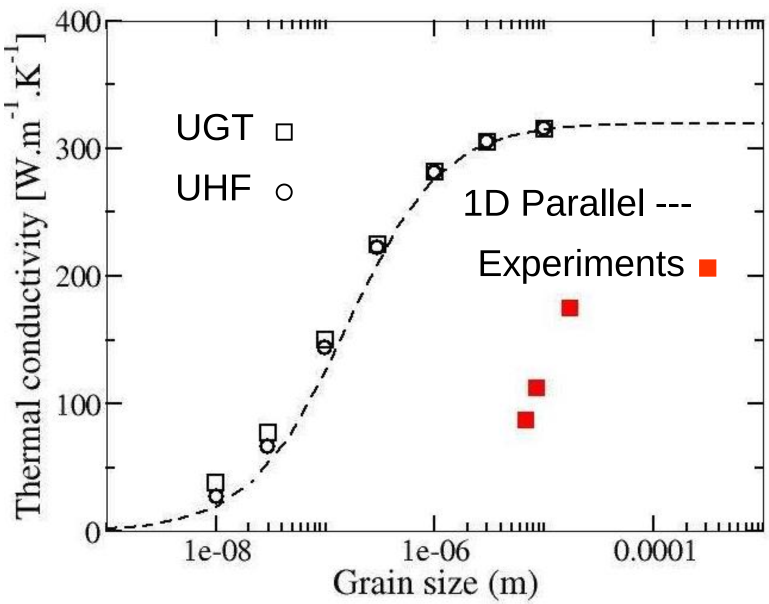


~400 grains

Effective (mean) behaviour



Mean grain size=10nm



Maximum relative difference (EF-1Dparallel)
-> less than 20%

Large discrepency with experimental results
-> too perfect grain boudaries in MD

Homogénéisation numérique : principes

Définition d'un chargement :

$$\begin{cases} div(\underline{\underline{\sigma}}) = 0 \\ \underline{\underline{\sigma}} = K : \underline{\underline{\varepsilon}} \\ (\underline{u}, \underline{\underline{\sigma}}.\underline{n})_{\partial\Omega} \in E_{X_0} \\ (\underline{u}, \underline{\underline{\sigma}}.\underline{n})_{\partial\Omega} \in E^{CL} \end{cases}$$

$(\underline{u}, \underline{\underline{\sigma}}.\underline{n})_{\partial\Omega} \in E_{X_0}$ ⟹ Chargement moyen

$(\underline{u}, \underline{\underline{\sigma}}.\underline{n})_{\partial\Omega} \in E^{CL}$ ⟹ Type de CL

Exemples de chargements moyens

$$E_{\Sigma_0} = \left\{ (\underline{v}, \underline{t})_{\partial\Omega} \middle/ \frac{1}{V} \int_{\partial\Omega} \underline{t} \otimes^s \underline{x} ds = \underline{\underline{\Sigma}}_0 \right\}$$

⟹ Contrainte moyenne = $\underline{\underline{\Sigma}}_0$

$$E_{E_0} = \left\{ (\underline{v}, \underline{t})_{\partial\Omega} \middle/ \frac{1}{V} \int_{\partial\Omega} \underline{v} \otimes^s \underline{n} ds = \underline{\underline{E}}_0 \right\}$$

⟹ Déformation moyenne = $\underline{\underline{E}}_0$

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Homogénéisation numérique : principes

Définition du comportement élastique apparent

A partir de 6 chargement linéairement indépendants*

(* pas de relation linéaire entre les 6 contraintes moyennes)

Approche mécanique

$$\overline{\underline{\underline{\sigma}}^{I}} = \tilde{K}^{mech} : \overline{\underline{\underline{\varepsilon}}^{I}}$$

Approche énergétique

$$\overline{e^{IJ}} = \overline{\underline{\underline{\sigma}}^{I} : \underline{\underline{\varepsilon}}^{J}} = \frac{1}{2}\overline{\underline{\underline{\varepsilon}}^{I}} : \tilde{K}^{ener} : \overline{\underline{\underline{\varepsilon}}^{J}}$$

Equivalence approche énergétique / approche mécanique

⇕

Tout chargement d'un « jeu de CL » doit respecter la condition de Hill

$$\frac{1}{2}\overline{\underline{\underline{\sigma}} : \underline{\underline{\varepsilon}}} = \frac{1}{2}\overline{\underline{\underline{\sigma}}} : \overline{\underline{\underline{\varepsilon}}} \quad \Longleftrightarrow \quad \int_{\partial\Omega} \left(\underline{t} - \overline{\underline{\underline{\sigma}}}.\underline{n}\right)\cdot\left(\underline{u} - \overline{\underline{\underline{\varepsilon}}}.\underline{x}\right) dS = \underline{0}$$

Homogénéisation numérique : principes

Les 3 « jeux de CL » classiques satisfaisant Hill

CL en Déformation Homogène au contour

$$E^{DH} = \left\{ (\underline{v},\underline{t})_{\partial\Omega} \Big/ \ \underline{v} = \overline{\underline{\underline{\varepsilon}}}.\underline{x} \ \left(avec \ \ \overline{\underline{\underline{\varepsilon}}} = \frac{1}{V} \int_{\partial\Omega} \underline{v} \otimes^s \underline{n} ds \right) \right\}$$

CL en Contrainte Homogène au contour

$$E^{CH} = \left\{ (\underline{v},\underline{t})_{\partial\Omega} \Big/ \ \underline{t} = \overline{\underline{\underline{\sigma}}}.\underline{n} \ \left(avec \ \ \overline{\underline{\underline{\sigma}}} = \frac{1}{V} \int_{\partial\Omega} \underline{t} \otimes^s \underline{x} ds \right) \right\}$$

CL Périodiques

$$E^{P} = \left\{ \begin{array}{l} (\underline{v},\underline{t})_{\partial\Omega} \Big/ \\ \underline{v}(\underline{x}+\underline{h}) = \underline{v}(\underline{x}) + \overline{\underline{\underline{\varepsilon}}}.\underline{h} \ \ et \ \ \underline{t}(\underline{x}+\underline{h}) = -\underline{t}(\underline{x}) \ \left(avec \ \ \overline{\underline{\underline{\varepsilon}}} = \frac{1}{V} \int_{\partial\Omega} \underline{v} \otimes^s \underline{n} ds \right) \end{array} \right\}$$