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Deformation in Semi-Crystalline Polymers from a Heterogeneous Spherulitic Microstructure

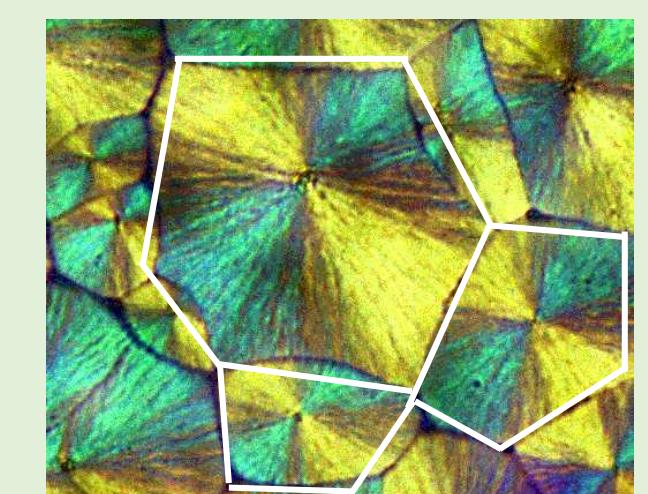
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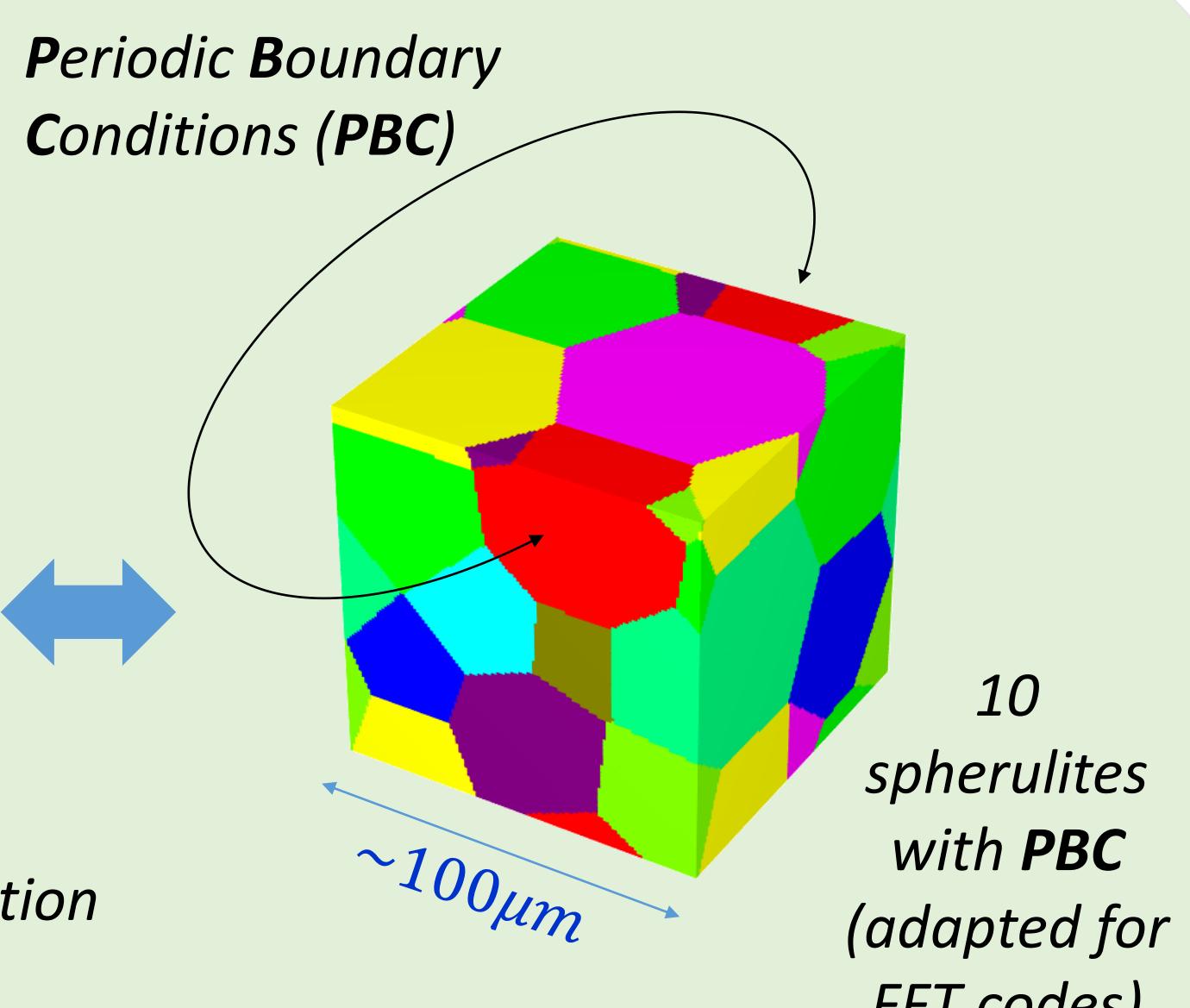
During a mechanical solicitation, the **microstructure of semi-crystalline polymers (PSCs)** such as High Density Polyethylene (HDPE), which have a **spherulitic structure**, evolves. Our objective is to **understand the micro-mechanisms of deformation** when the solicitation remains in the low deformation range but takes into account the **viscoelastic character** of the amorphous phase. We will use a code based on the **resolution of the Lippman-Schwinger equations by Fourier transform** (*H. Moulinec, P. Suquet, Comput. Methods Appl. Mech. Engrg. 1998, 157, 69-94*; use of code [AMITEX](https://amitexftp.github.io/AMITEX/index.html) developed at CEA Saclay - <https://amitexftp.github.io/AMITEX/index.html>).

1 Conception of an ideal 3D spherulitic microstructure

Several Spherulites :
"Multi-grain like" structure

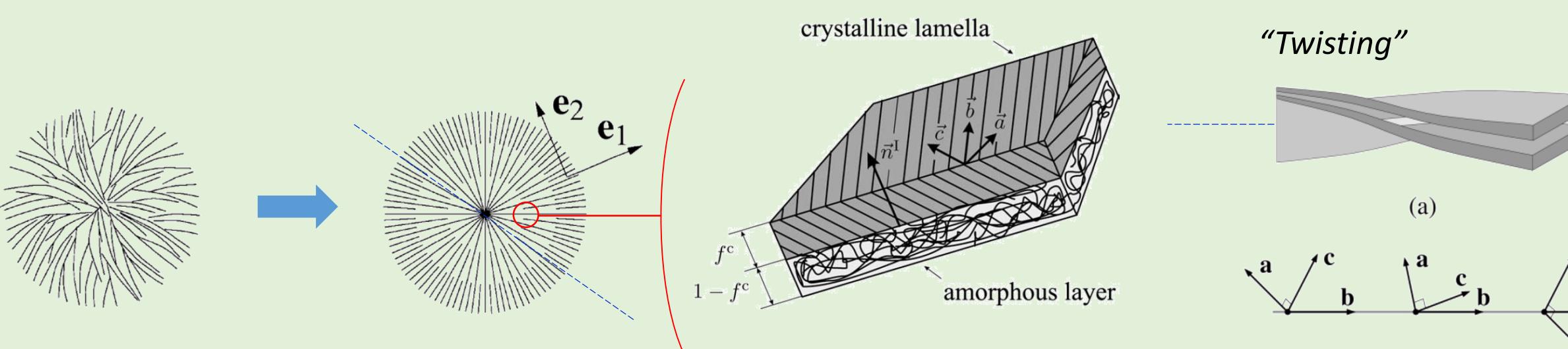


Neper tool : Polycrystal Generation and Meshing (<https://neper.info/>)



Model for 1 spherulite

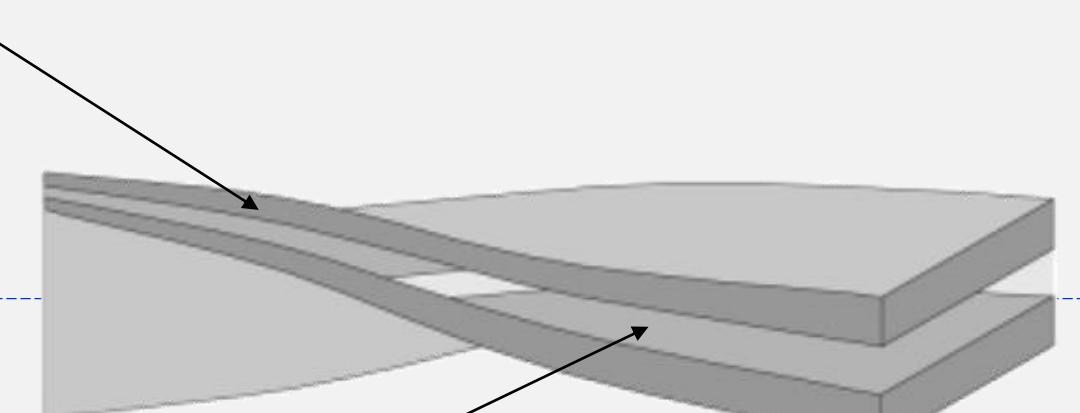
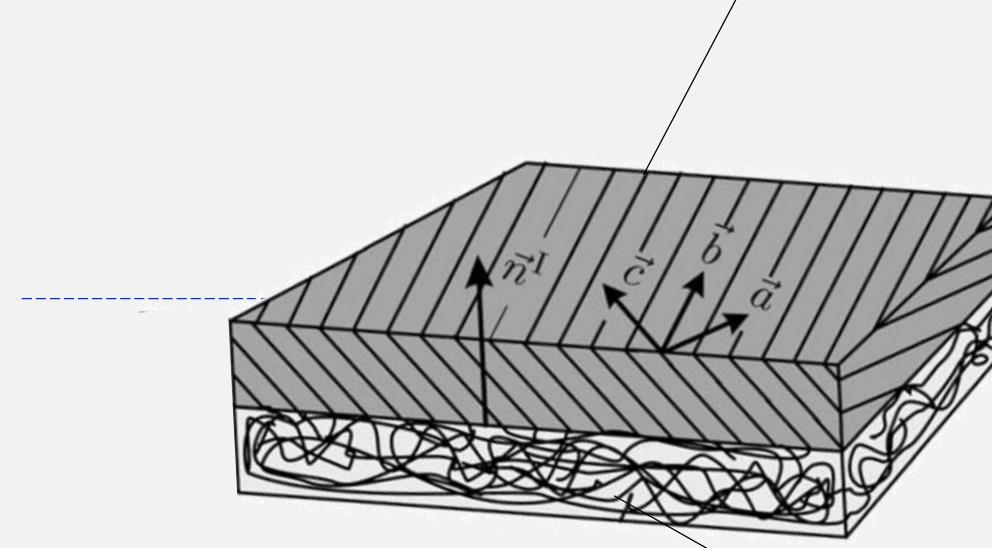
[Allan P. Bevis M.
Phil. Mag. 1977, 35,
405-30]



Micromechanical model of a two-layer lamella in High Density Poly-Ethylene (HDPE)

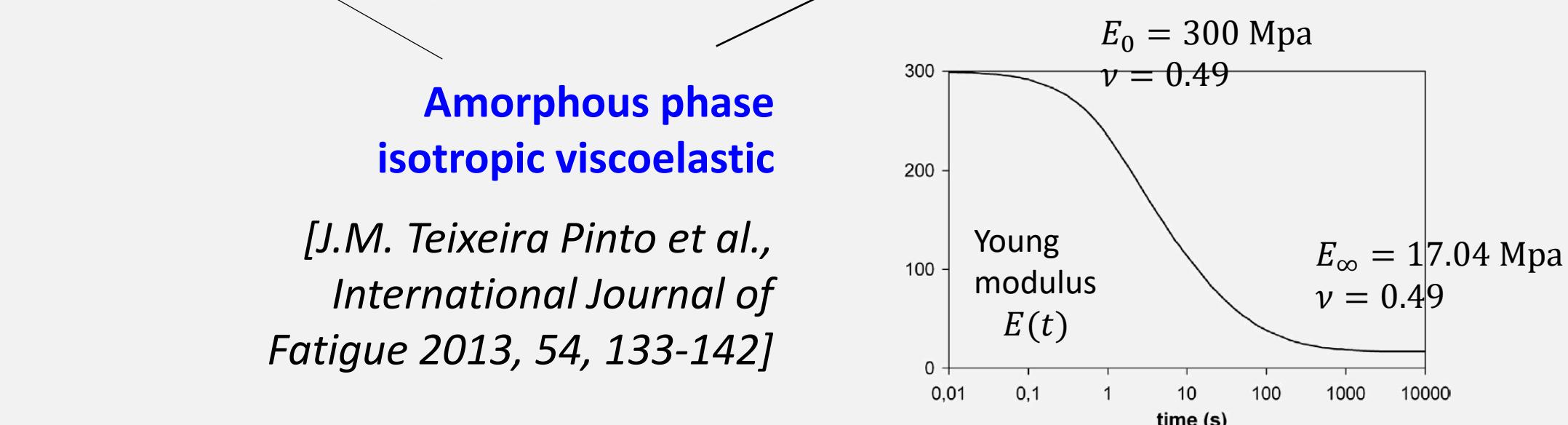
Orthotropic elastic crystal

C₁₁ 7.99 C₂₂ 9.92 C₃₃ 315.92 C₁₂ 3.28 C₁₃ 1.13 C₂₃ 2.14 C₄₄ 3.62 C₅₅ 1.62 C₆₆ 3.19 [Tashiro, K.; Kobayashi, M.; Tadakoro, H. Macromolecules 1978, 11, 914-918.]



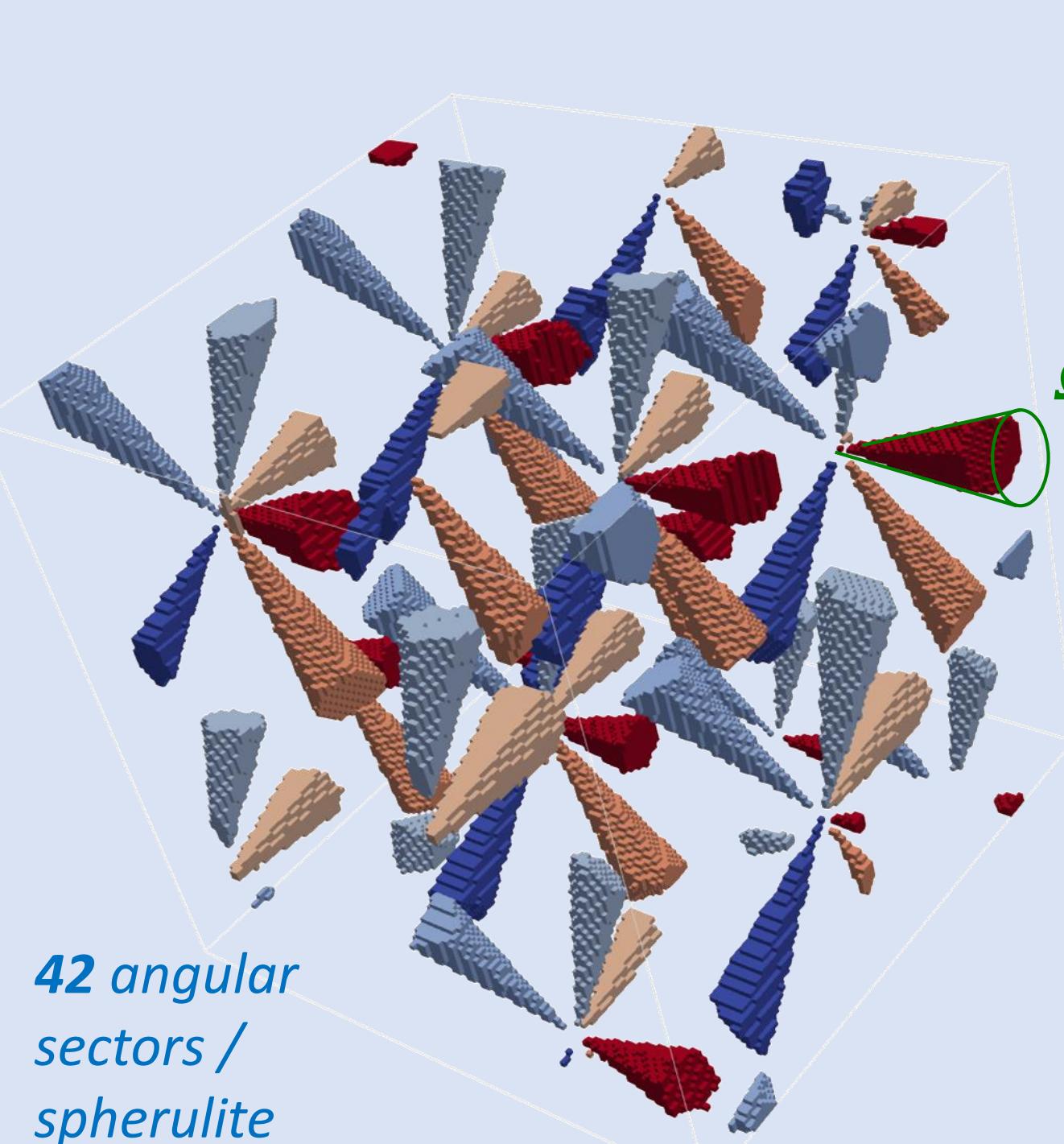
Amorphous phase isotropic viscoelastic

[J.M. Teixeira Pinto et al., International Journal of Fatigue 2013, 54, 133-142]



2 Development

of a specific viscoelastic behavior law for spherulitic microstructures



A Each spherulite is cut into equivalent angular sectors Ω

B for each sector : transverse isotropic viscoelastic behavior

(70% crystal / 30% amorphous)

5 instantaneous moduli $M_{i,instant}$ (short times)

5 relaxed moduli $M_{i,relax}$ (long times)

5 relaxation times $\tau_{i,relax}$

Tool : [AMITEX](https://amitexftp.github.io/AMITEX/index.html) (FFT code)

Transverse isotropic elastic stiffness matrix (Voigt notation)

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & \\ C_{22} & C_{23} & C_{33} & C_{44} & \\ C_{33} & C_{66} & 0 & C_{55} & \\ sym & & & C_{55} & C_{66} \\ \eta & l & l & G_{12} & G_{12} \\ K_{23} + G_{23} & K_{23} - G_{23} & K_{23} + G_{23} & G_{12} & G_{23} \\ sym & & & G_{12} & G_{23} \end{bmatrix} = \eta + l + K_{23} + G_{23} + G_{12}$$

[N. Zobeiry et al., Mechanics of Materials 2016, 97, 76-91]

transverse isotropic viscoelastic law

$$\dot{\sigma} = \sum_{i=1}^5 \dot{\sigma}_i = \sum M_{i,instant} \dot{\epsilon}_i - \frac{\sigma_i - M_{i,relax} \epsilon_i}{\tau_{i,relax}}$$

$$M_i = \eta, l, K_{23}, G_{23}, G_{12}$$

3 Mechanical response and stress distribution in spherulites under basic loading

Tool : [AMITEX](https://amitexftp.github.io/AMITEX/index.html) (FFT code)

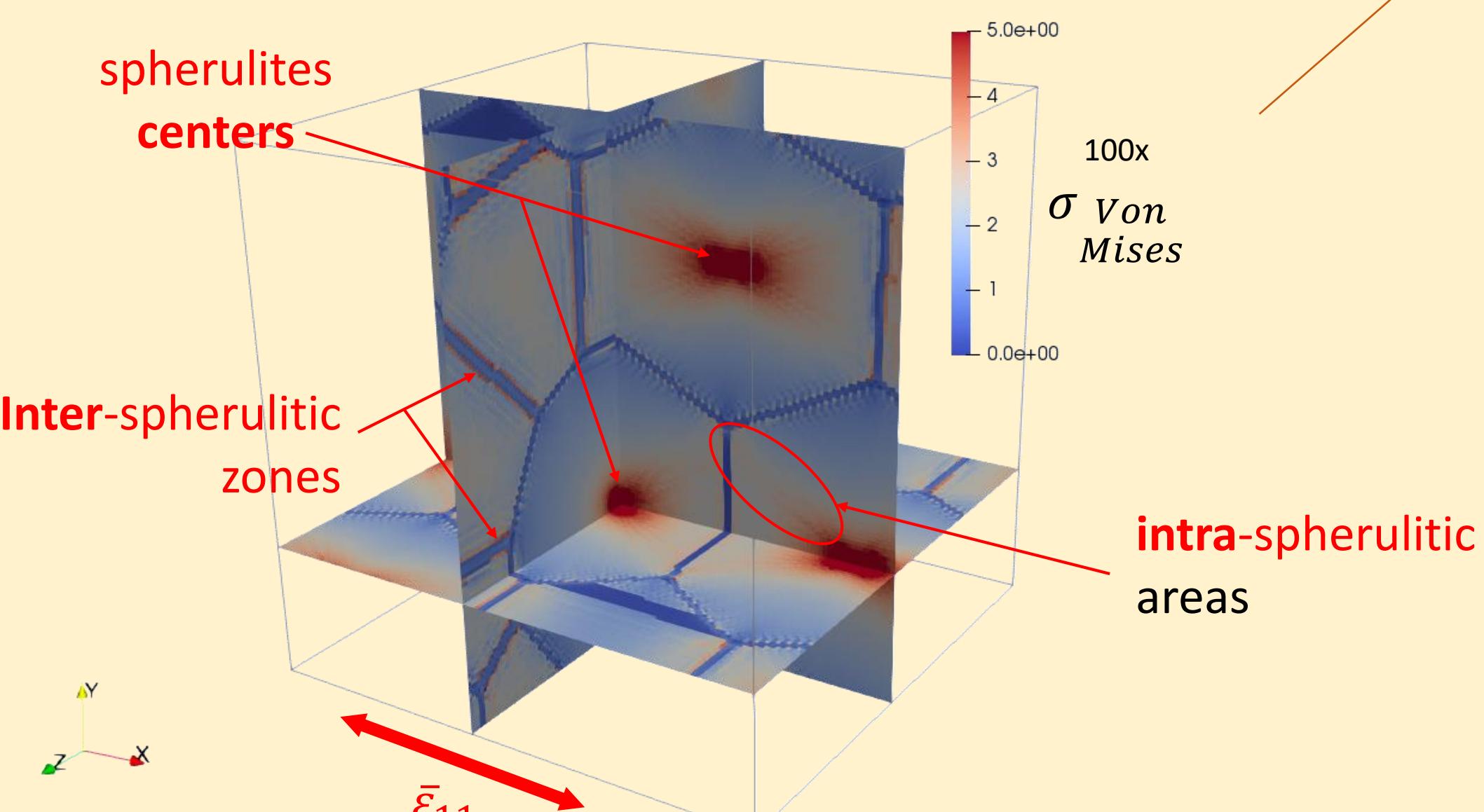
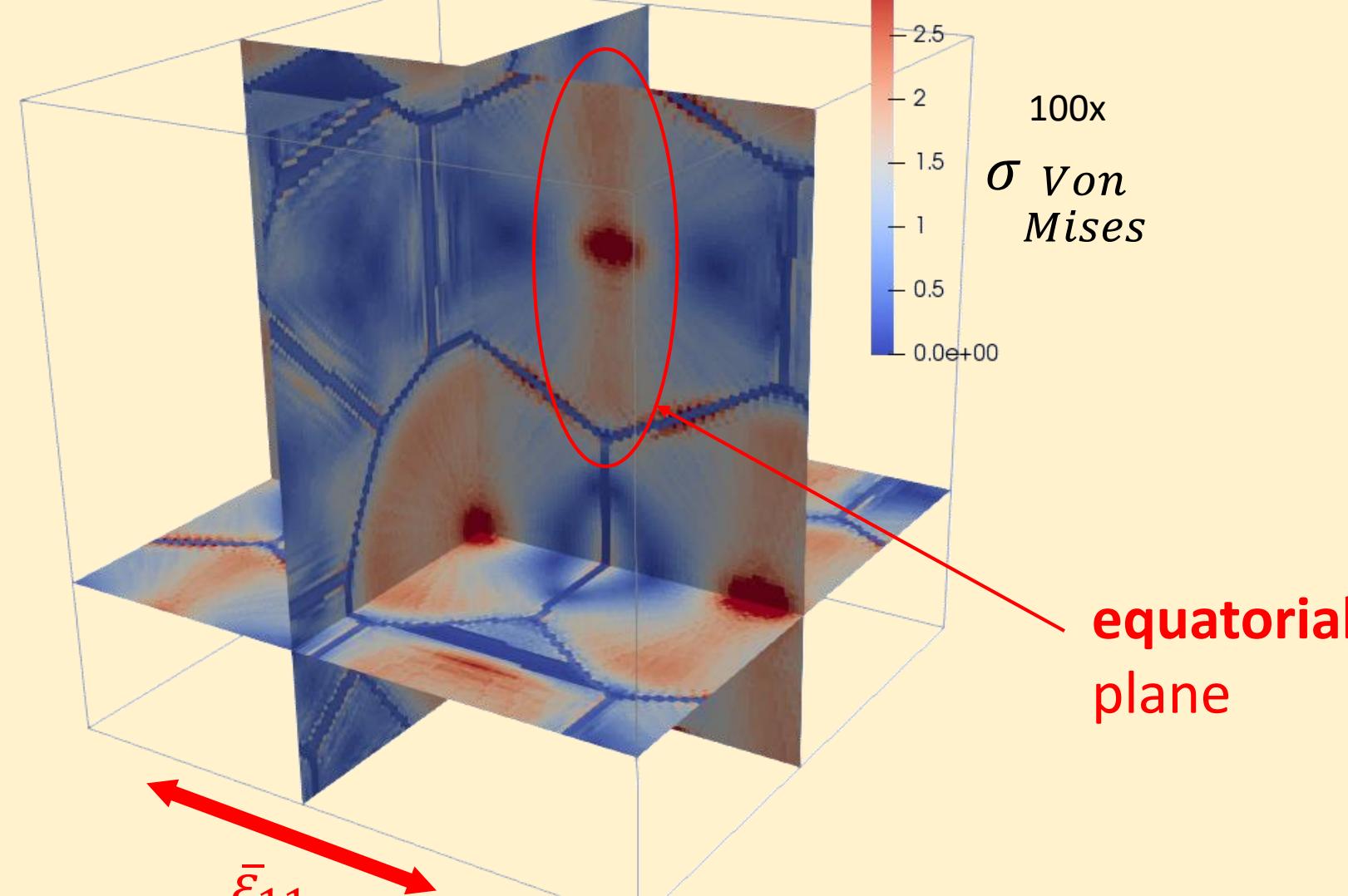
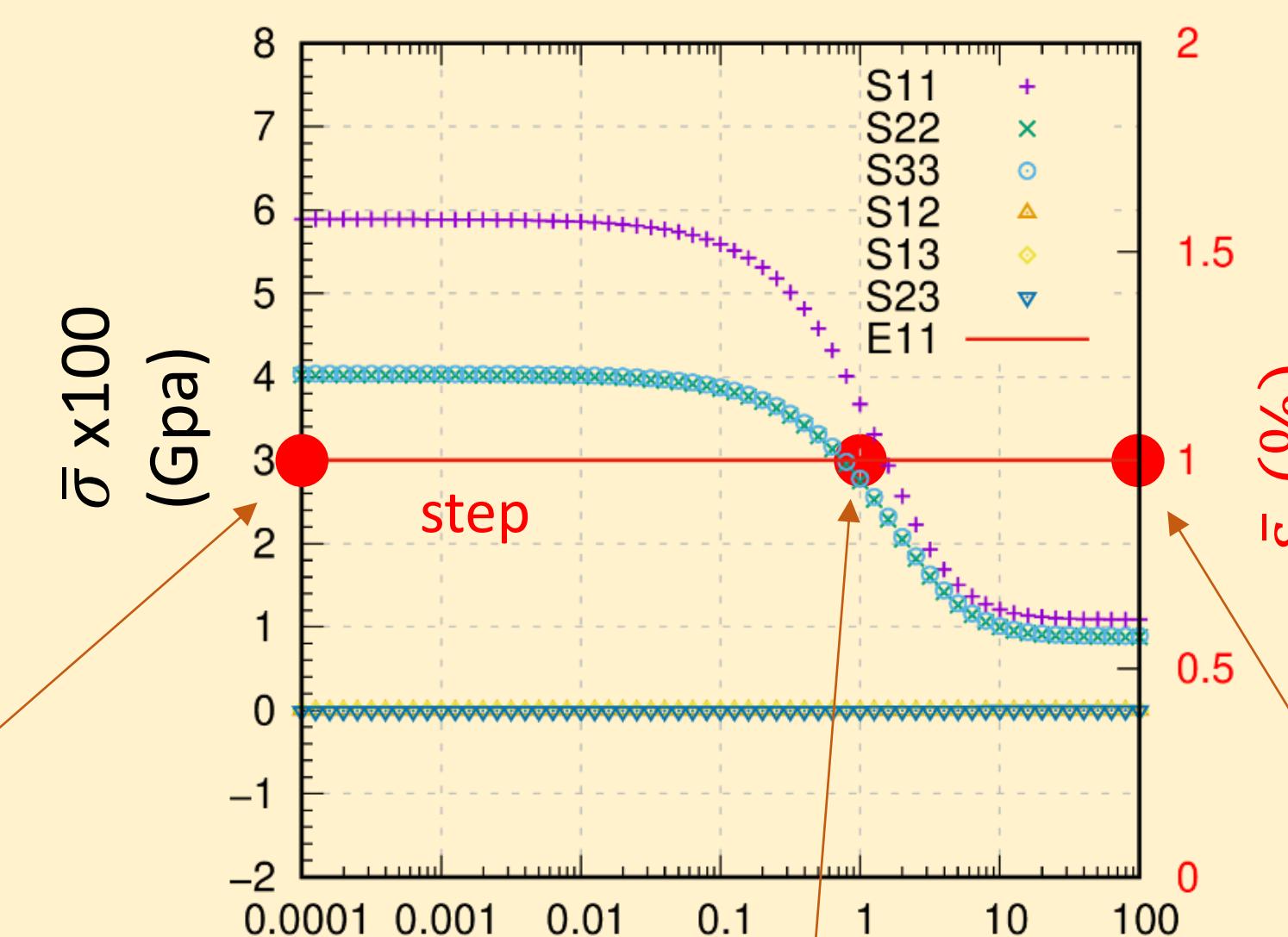
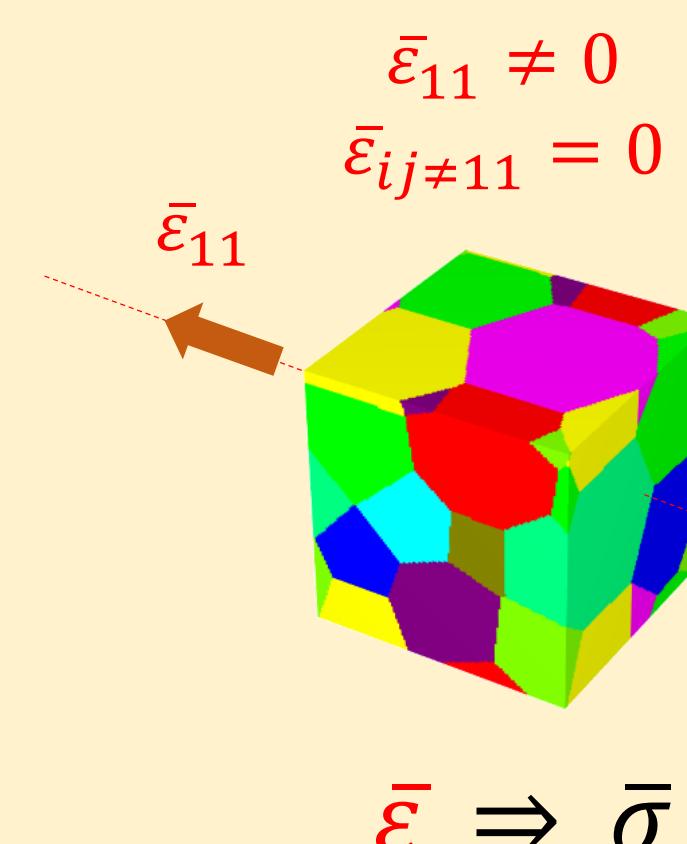
Behavior law numerical Format : UMAT
Behavior law numerical scheme : semi-analytic

642 angular sectors / spherulite

10 spherulites

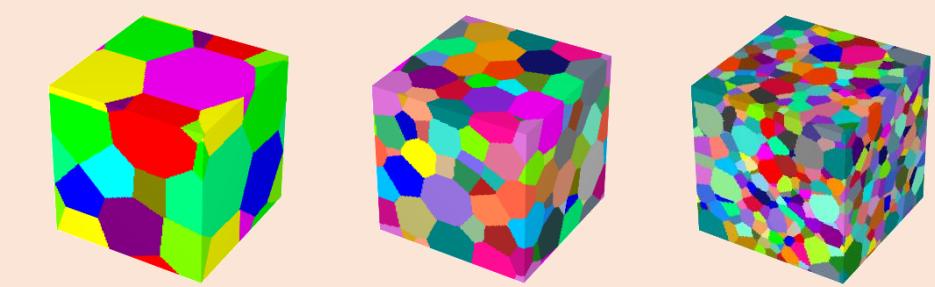
Inter-spherulitic behavior : amorphous

Inter-spherulitic thickness : ~ 1-2 microns

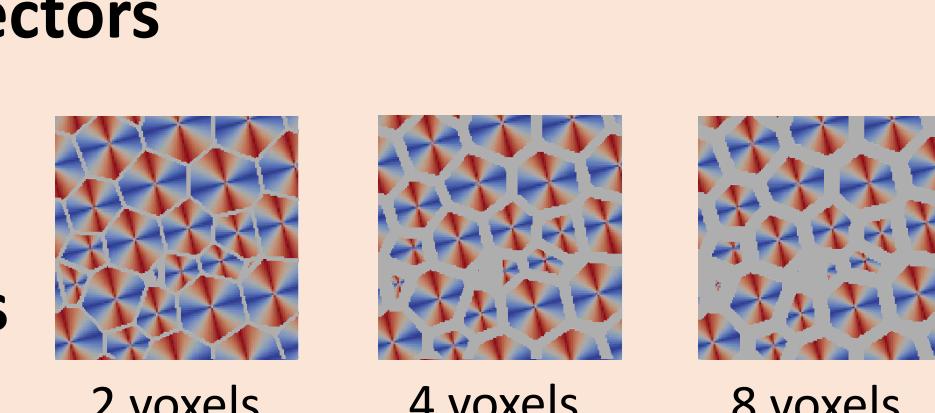


... undergoing work

□ Size distribution

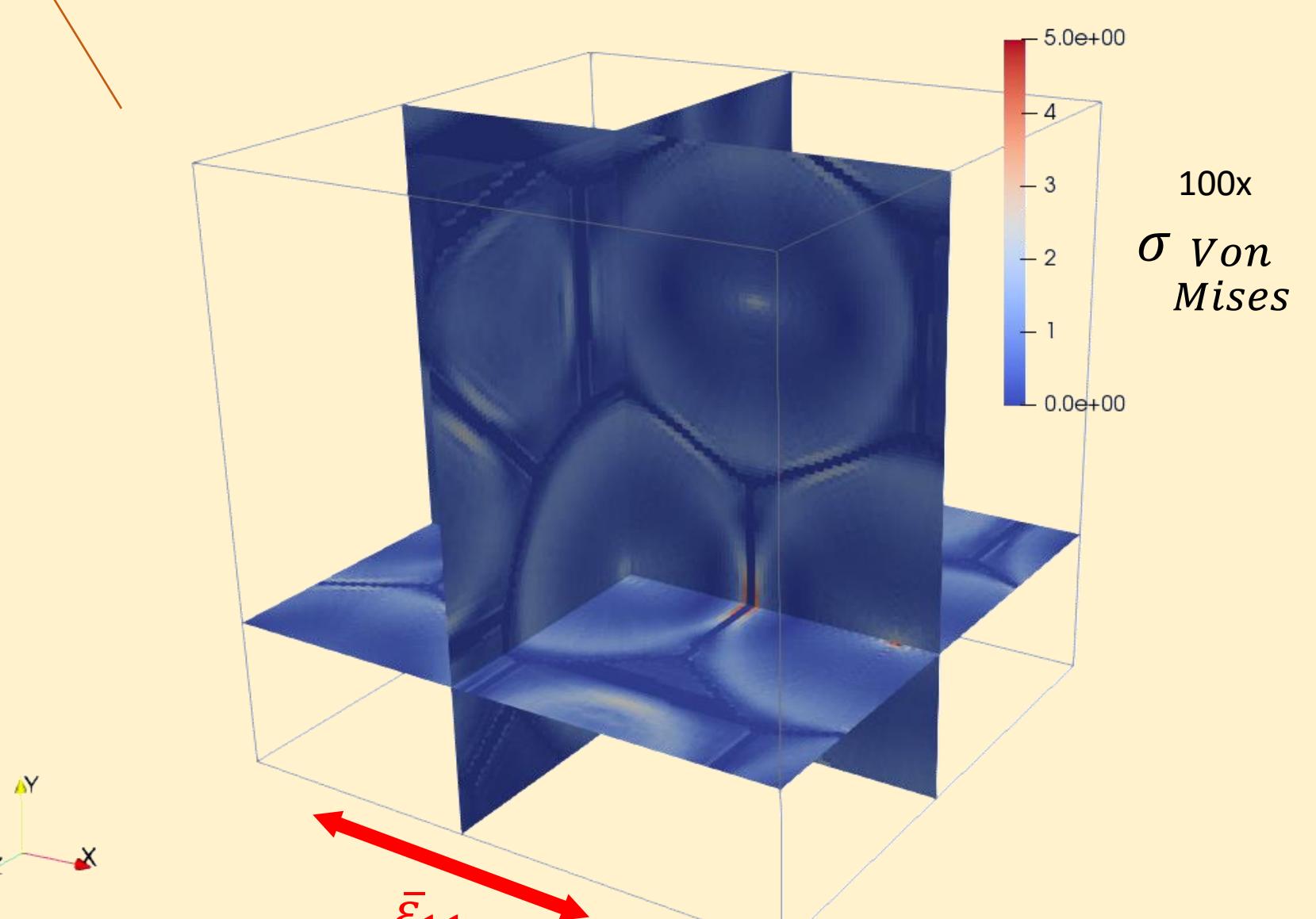


□ Number of angular sectors



□ Volume fraction of inter-spherulitic zones

□ Dynamical Mechanical Analysis - Experimental and virtual DMA [S. André, J. Boisse, C. Noûs, JTCAM 2021]



Conclusion

- Conception of spherulitic distributions with NEPER
- Decomposition of spherulites into angular sectors with a transverse isotropic viscoelastic behavior

- Identification of relaxed / instantaneous moduli
- Implementation of a transverse isotropic viscoelastic law in UMAT format
- First mechanical simulations with AMITEX