# Seminar – Thiebaud Richeton (LEM3, Metz)

**Monday, December 17th 2018, 2pm**
**Amphi 100, campus Artem**

## Media with heterogeneous elasticity: elastic fields due to dislocation pile-ups at finite grain boundaries and mechanical derivations of elastic constants of ε-martensite

T. Richeton, X. Chen, S. Berbenni

Dislocations especially interact with grain boundaries through their elastic fields. In media with heterogeneous elasticity, image stresses are indeed appended to the self dislocation stress field in order to satisfy boundary conditions. Moreover, real grain boundaries have finite width and their specific elasticity may then constitute an additional source of image forces. This presentation will deal with elastic fields due to single dislocations and dislocation pile-ups, computed thanks to the Eshelby-Stroh-Leknitskii formalism for two-dimensional anisotropic elasticity, in bi-materials, half-spaces and tri-materials so as to consider finite grain boundary regions. In particular, effects of grain boundary stiffness and grains misorientation on Peach-Koehler forces, pile-up lengths and stress concentrations in neighboring grain will be analyzed. Also, the role of image forces on grain boundary mobility will be discussed. The second part of the presentation will be dedicated to the mechanical derivations of anisotropic elastic constants of HCP ε-martensite, considered as a periodic laminate structure composed of alternating twinned and untwinned phases, from FCC austenite elastic constants. The consequence of this elastic heterogeneity on mechanical properties will be discussed.

## Local speaker - Komlavi Senyo ELOH (304)

## Fast Fourier Transform simulation of X-Ray diffraction peaks of single crystals and polycrystals: application to reference cases

Komlavi Senyo ELOH, Alain JACQUES, Stéphane BERBENNI

A new expression of the periodized discrete Green operator using the Discrete Fourier Transform method and consistent with the Fourier grid is derived from the classic "Continuous Green Operator" in order to avoid the problem referred to as "aliasing" inherent to Discrete Fourier Transform methods. It is shown that the easy use of the conventional continuous Fourier transform of the modified Green operator for heterogeneous materials with eigenstrains leads to spurious oscillations when computing the local responses of composite materials close to materials discontinuities like interfaces, dislocations, edges. We also focus on the calculation of the displacement field and its associated discrete Green operator which may be useful for materials characterization methods like X- ray diffraction techniques. The development of these new consistent discrete Green operators in the Fourier space allows to eliminate oscillations while retaining similar convergence capability. For illustration, the new discrete Green operators are implemented in a fixed-point algorithm for heterogeneous periodic composites knows as the Moulinec and Suquet (1994,1998) "basic scheme" that we extended to consider eigenstrain fields, as in Anglin, Lebensohn and Rollett (2014). Artifacts due to voxelisation which appear on the displacement field in the case of inclined dislocation loop, are also removed using a “subvoxelization” method. We will show the effect of these defects (oscillations and artifacts) on the displacement field and the diffraction peaks as well as their correction, in the case of a homogeneous medium with an inclined dislocation loop.