INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

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Prof. Theodore Karakasidis
Department of Civil Engineering
University of Thessaly, Volos, Greece

A multi-scale numerical model for crack propagation in a matrix with inclusions

It is well known that crystalline inclusions affect the mechanical properties of materials. A semi-analytical model has been developed in two-dimensions in order to describe the observed behaviour of crack propagation related with a standalone inclusion, which is in good agreement with the observed behaviour [1]. However, the description of the collective effect of crystalline inclusions on crack propagation as function of concentration, size as well as cohesion energies of matrix and inclusions is very difficult to treat analytically. The available common simulation methods present several drawbacks due to the fact that crack propagation is a multiscale phenomenon. Finite Elements permit to simulate large samples, however the continuum approach is not valid at very small scales. On the other hand Molecular Dynamics which describes materials at the atomic scale is very computationally intensive.

Thus we developed a two dimensional coarse-grained computational approach where the material is separated in small blocks and where we have square crystallites which are surrounded by a grain boundary region. A methodology was developed for creation of material samples with given concentration of crystalline materials and with a tailored distribution of crystallite sizes. The different blocks are characterized by the corresponding cohesion energy of the materials (matrix, crystalline inclusions and grain boundary zone). A crack is initiated with a given energy and a block of material is broken based on probabilistic arguments, using a modified random walker with a preferred direction. Several crack propagations are performed on a given digital sample and quantities such the mean length of the crack and its velocity are obtained. This way we investigated in a first place the effect of crystalline inclusion material concentration as well as the effect of the size of the crystallites, as well as the effect of the difference of cohesive energies of the matrix and the crystalline inclusion. An important outcome is also that when dealing with small size crystallites on has to take into account the modification of the cohesive energy compared to that of the bulk. The results seem to be in qualitative agreement with the literature results and thus the model seems to be quite promising since can be used with some extensions as an efficient hierarchical simulation methodology, with input either from experimental results or classical/ab-initio-molecular dynamics methods.

References:
[1] Charitidis, C. A., Karakasidis, T. E., Kavouras, P., & Karakostas, T. (2007). Journal of Physics: Condensed Matter, 19(26), 266209.