

# Failure Mechanism in Materials and Meso-Scale Structures

## Opportunity

Materials degradation and failure is a fundamental problem in engineering and nanotechnology. The definition of failure of a particular structure and material is unclear and ill-defined. Experimental measurements on failure are difficult and widely scattered. Computational approach based on recent development can accelerate the progress.

## Meso Challenge

Understanding degradation and failure is at the heart of meso-scale challenge and could be ultimately traced to the atomistic origin of the material. Laboratory measurements on failure could be greatly benefited from large scale simulations based on exascale ( $10^{18}$ ) super-computing technology. The challenge is to properly link the computed data, the measured data and the underlining interactions at the meso-scale.

References: G.N. Greaves, et al, Nature Materials, 10, 2011, p823; R.O. Ritchie, Nature Materials, 10, 2011, p817.

## Approach

The approach used should incorporate the experimentalists, instrument developers, computational scientists and mathematicians working closely together. Extensive collection into databases for datamining of degradation and failure mechanisms and the resulting damage accumulation for different materials under different conditions is of paramount importance.

## Impact

The impact of understanding and more precisely defining failure mechanisms can accelerate the progress of materials design and choice. It will impact industries ranging from steels and concretes for buildings, to biomedical devices based on Viral Nanoparticles, as well as to fundamental advances in basic science and engineering.