

ABSTRACT

The fracture properties, in particular the ductility, of shale rocks is a key parameter for the engineering of hydraulic fracturing. We use molecular simulations to estimate fracture properties of shales constituents at the nanometer scale. First, we develop a methodology to estimate fracture properties by molecular simulation based on a thermodynamic integration. We validate the methodology on the specific case of silica for which experimental data are available and the classical theory of Linear Elastic Fracture Mechanics (LEFM) is valid. Then, we apply the methodology to a microporous carbon, which is a rough representation of kerogen at the molecular scale. We identify a significant ductility and we show that LEFM could not apply to kerogen at least at the nanometer scale. Finally, we reconstruct the silica-kerogen interface based on quantum calculation and we estimate its fracture properties. As for bulk kerogen, we identify a significant ductility. Finally, we present some up-scaling scenarios, which show that a small fraction of kerogen can turn a brittle mineral matrix into ductile heterogeneous shale.

CONTEXT

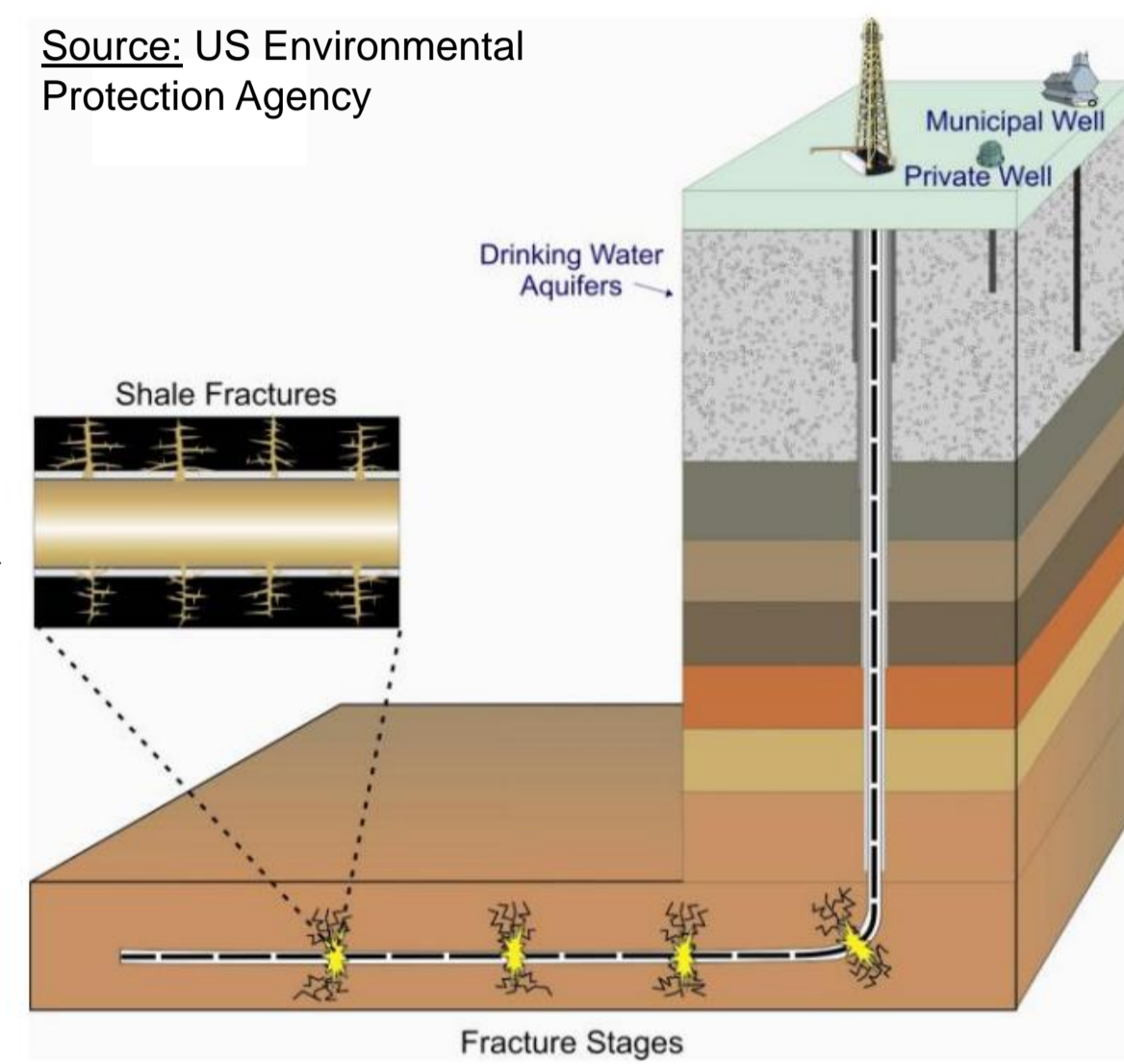
While conventional oil/gas is produced from permeable reservoir rock, shale gas is produced from almost impermeable source rock, and industry performs hydraulic fracturing to enhance oil/gas recovery. Ductility of shale rock plays a key role in crack propagation

- Brittle shales “shatter”, leading to a vast array of small-scale induced fractures providing numerous flow paths. Fracturing is performed with usual slick water and low proppant concentration.

- Ductile shale deform instead of shattering, leading to relatively few induced fractures and providing only limited flow paths. Fracturing requires complex fluids and high proppant concentration.

Clay and kerogen are known to increase the ductility of shales, but laboratory experiments at the scale of clay and kerogen particle is very challenging.

Objective: study the role of kerogen in the ductility of shale from the molecular scale and develop a fine understanding of the fracture properties of shales

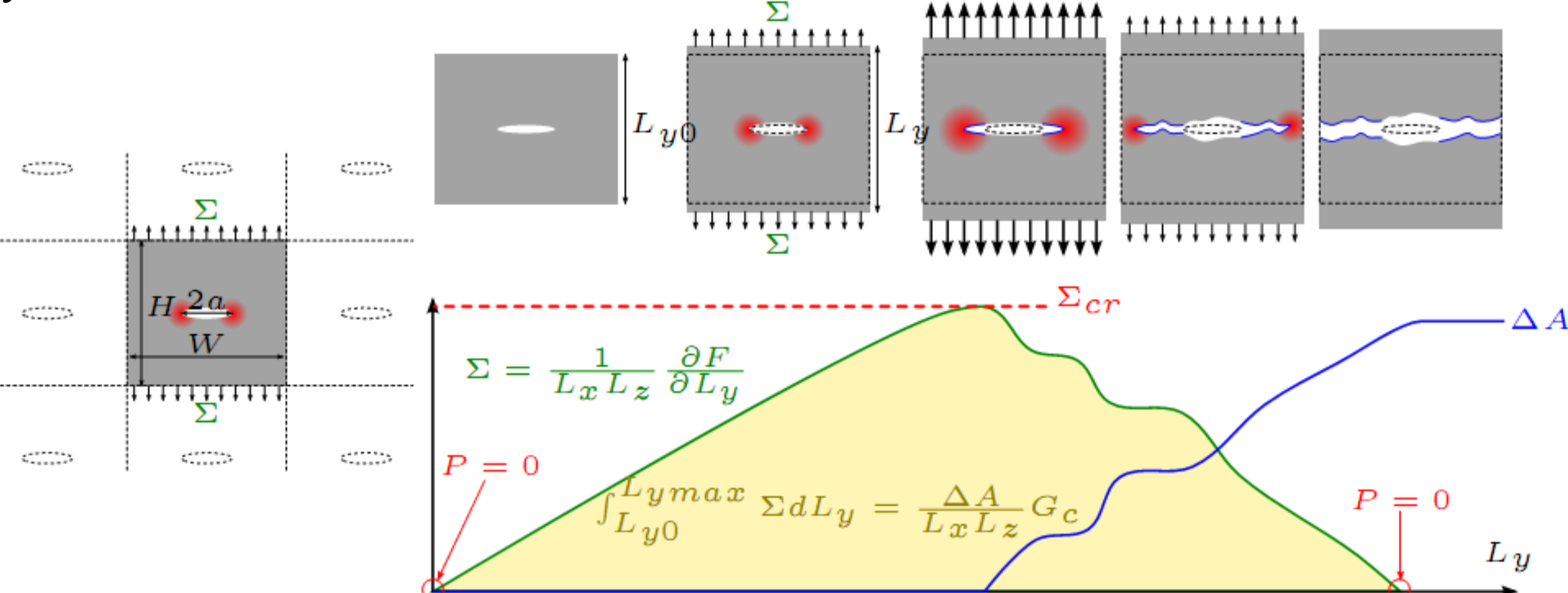


METHODOLOGY AND VALIDATION WITH SILICA

Methodology

Thermodynamic integration is used to estimate the energy release rate G_c of a material by molecular simulation

- Periodic through crack
- Stretch progressively (L_y)
- Compute the average stress Σ
- Integrate the stress over the strain



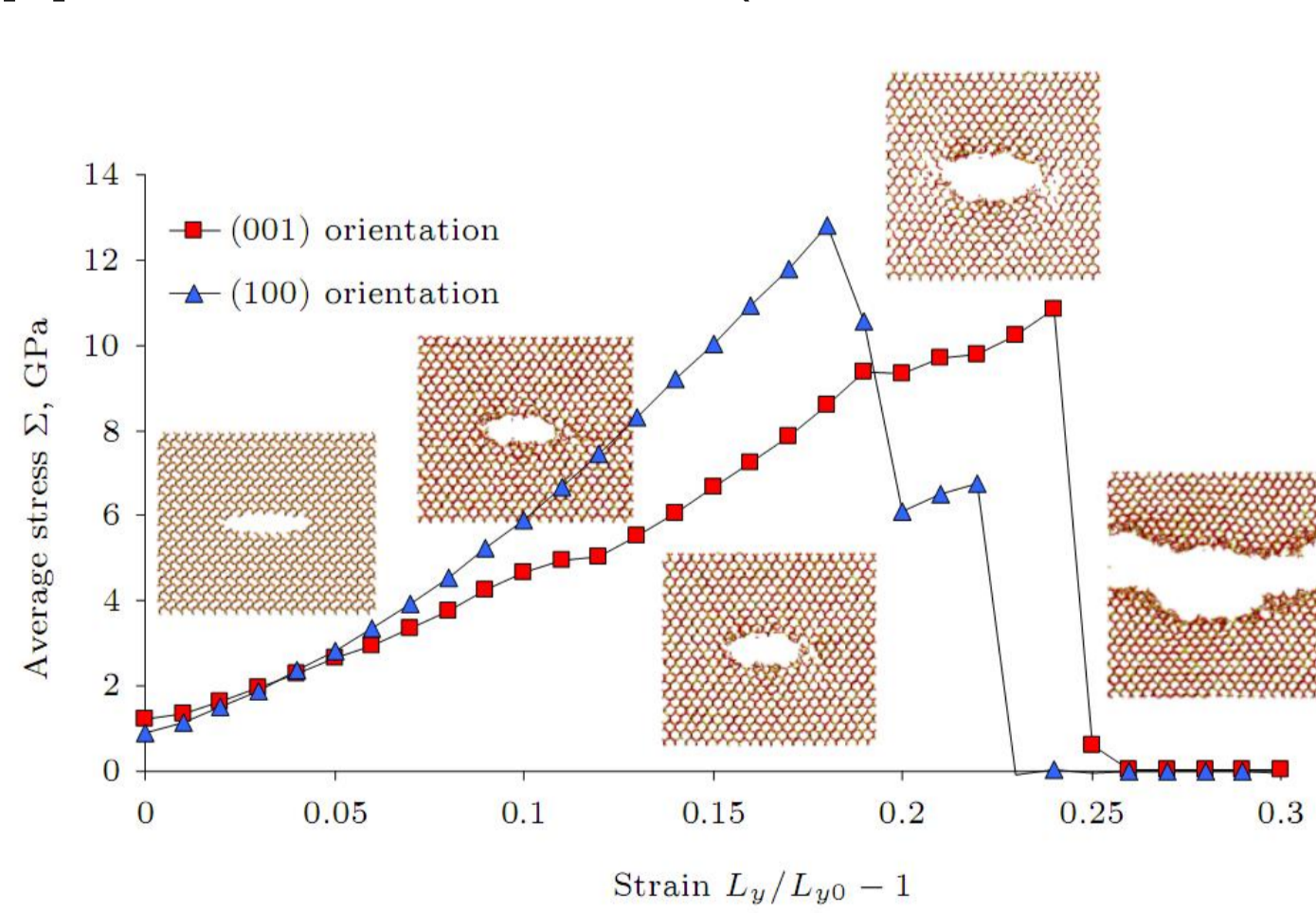
Another classical route consists in estimating the fracture toughness K_{Ic} from the critical stress Σ_{cr} assuming that the theory of Linear Elastic Fracture Mechanics (LEFM) is valid (brittle linear elastic material)

$$\Sigma_{cr} = \frac{K_{Ic}}{\sqrt{\pi a C}} \left(\frac{a}{W}, \frac{H}{W} \right) = \frac{K_{Ic}}{\sqrt{\pi a_{eff}}}$$

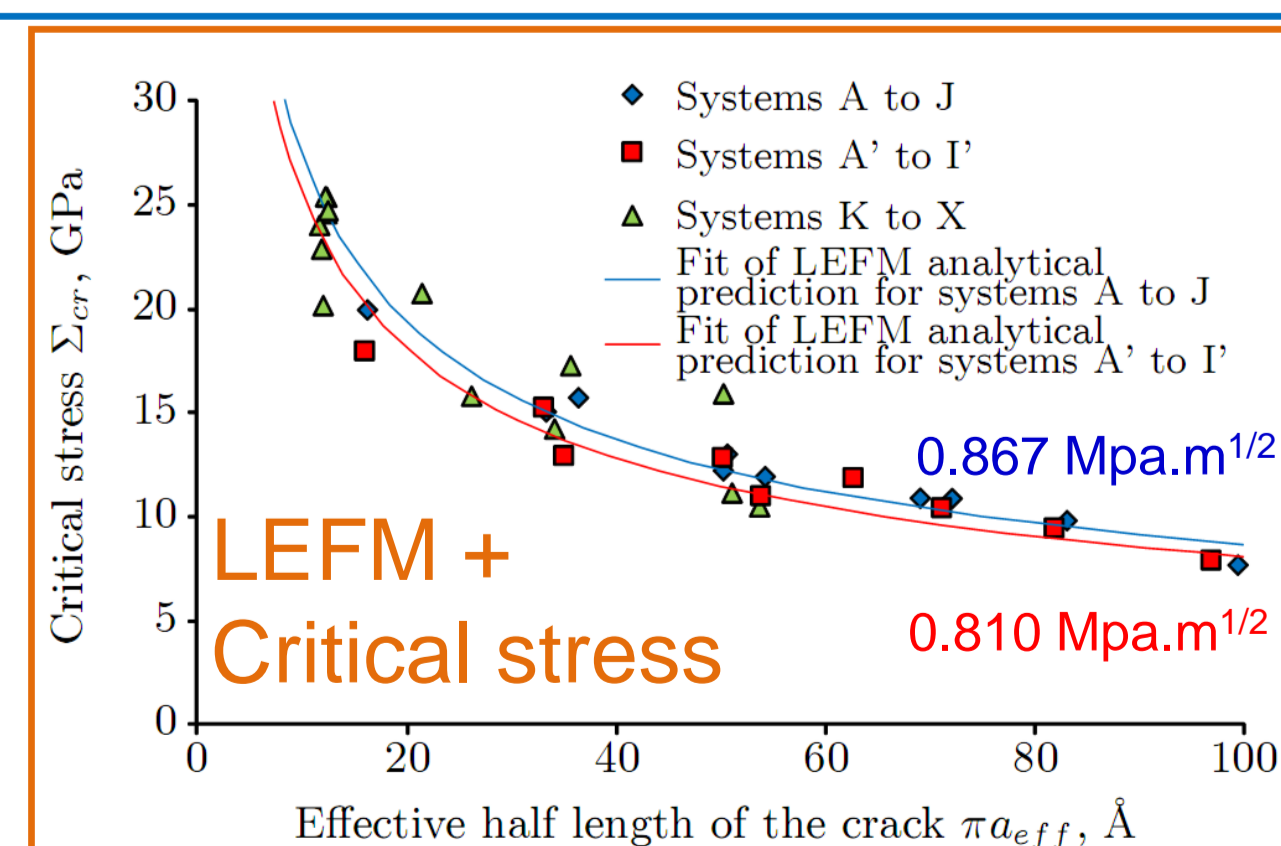
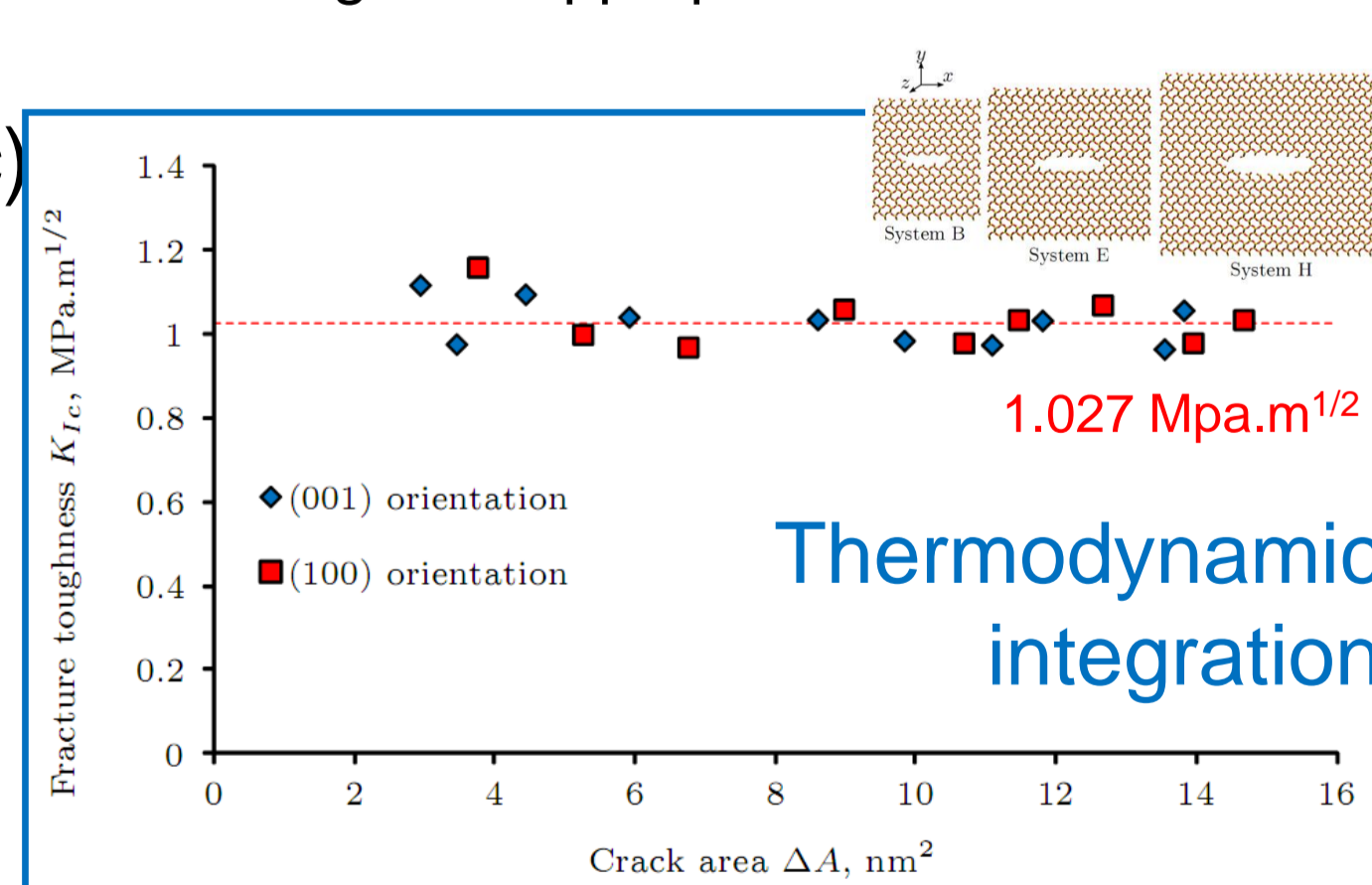
Toughness K_{Ic} and energy release rate G_c related through the appropriate Irwin's formula

Numerical estimation of G_c : Karimhaloo et al., *Journal of the Mechanics and Physics of Solids* (1996) 44:1565

Application to silica (brittle linear elastic)



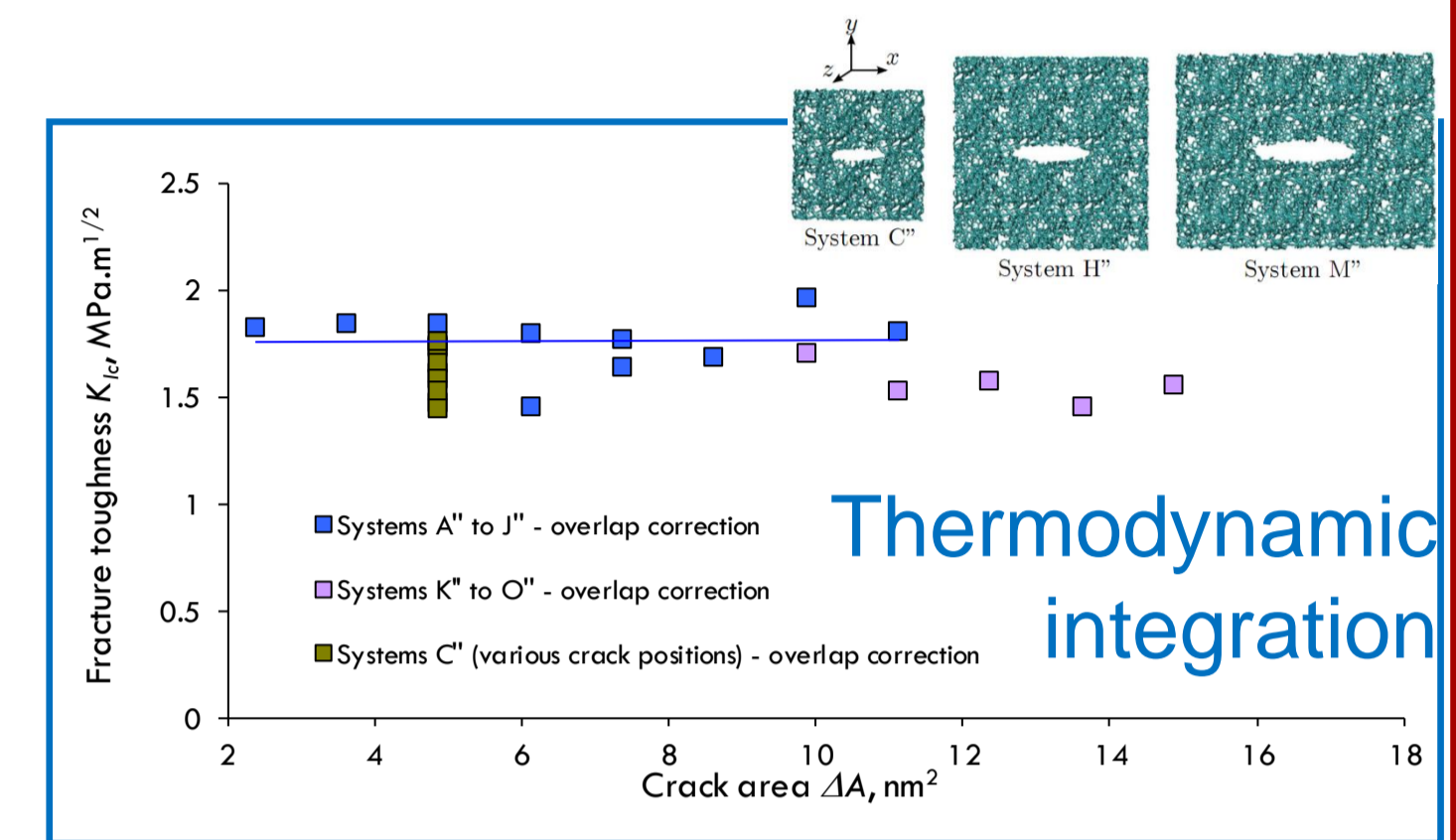
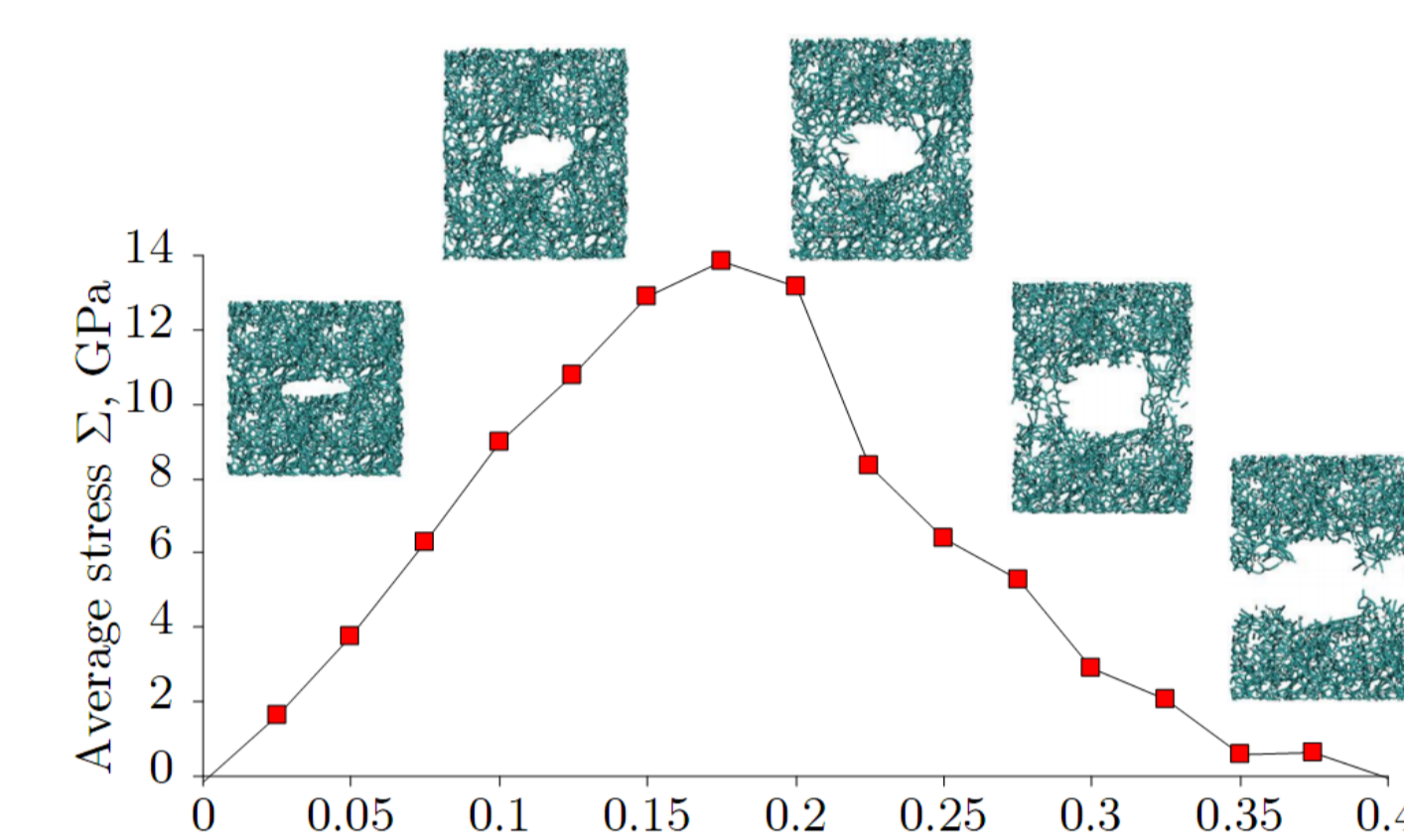
Both routes are valid and lead to similar results. Those results are consistent with experimental results available in the literature (Lucas J et al. *Scripta Metall Mater* 1995;32:743) : $0.82 \text{ Mpa.m}^{1/2}$



APPLICATION TO KEROGEN AND KEROGEN-SILICA INTERFACE

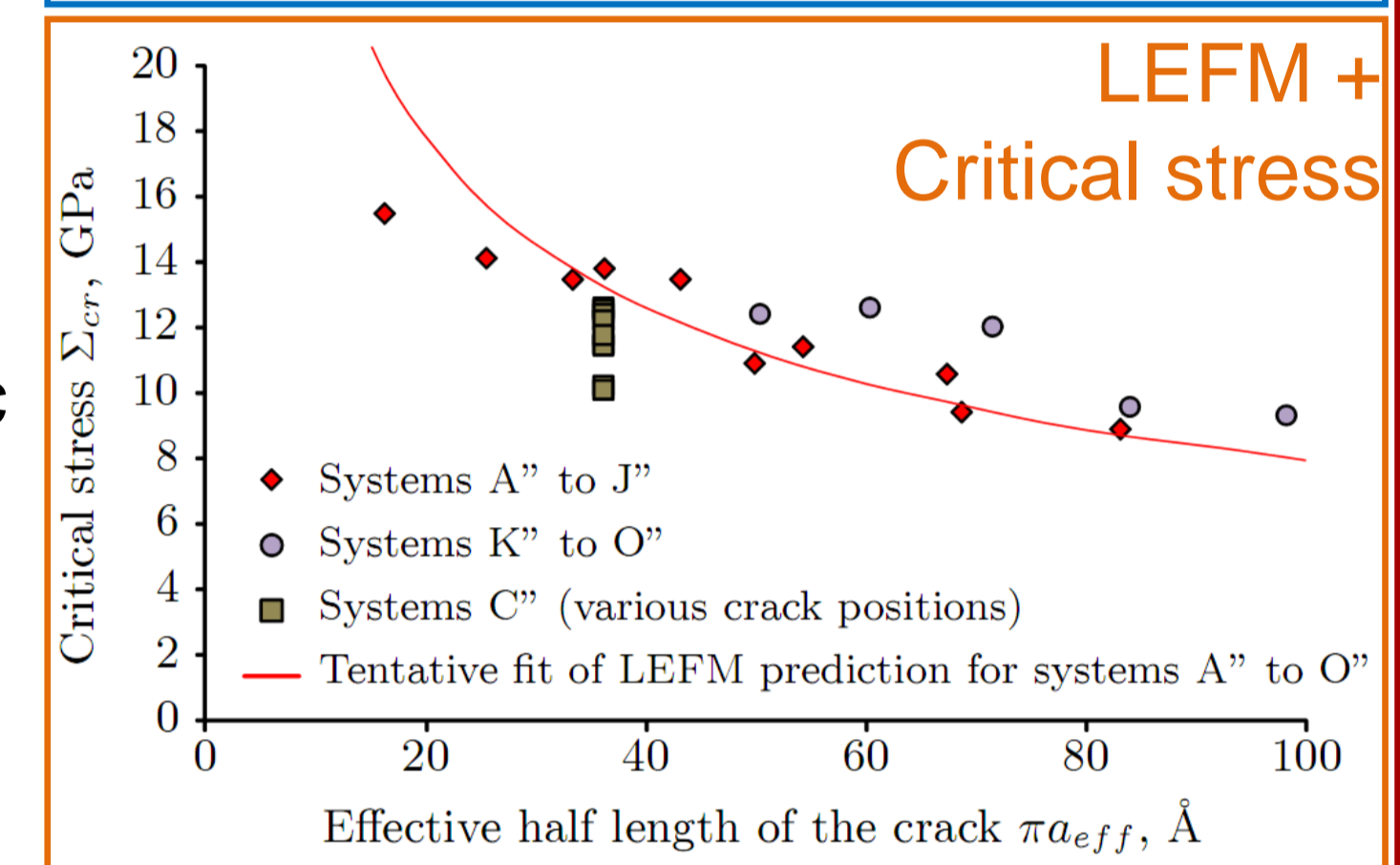
Bulk kerogen

Kerogen, the organic part of shale, is a disordered meso- and micro-porous carbon (like coal, activated carbons etc.) with significant H and O content. We study a typical micro-porous carbon molecular structure, CS1000, which is similar to the matrix of very mature kerogen without the mesopores.

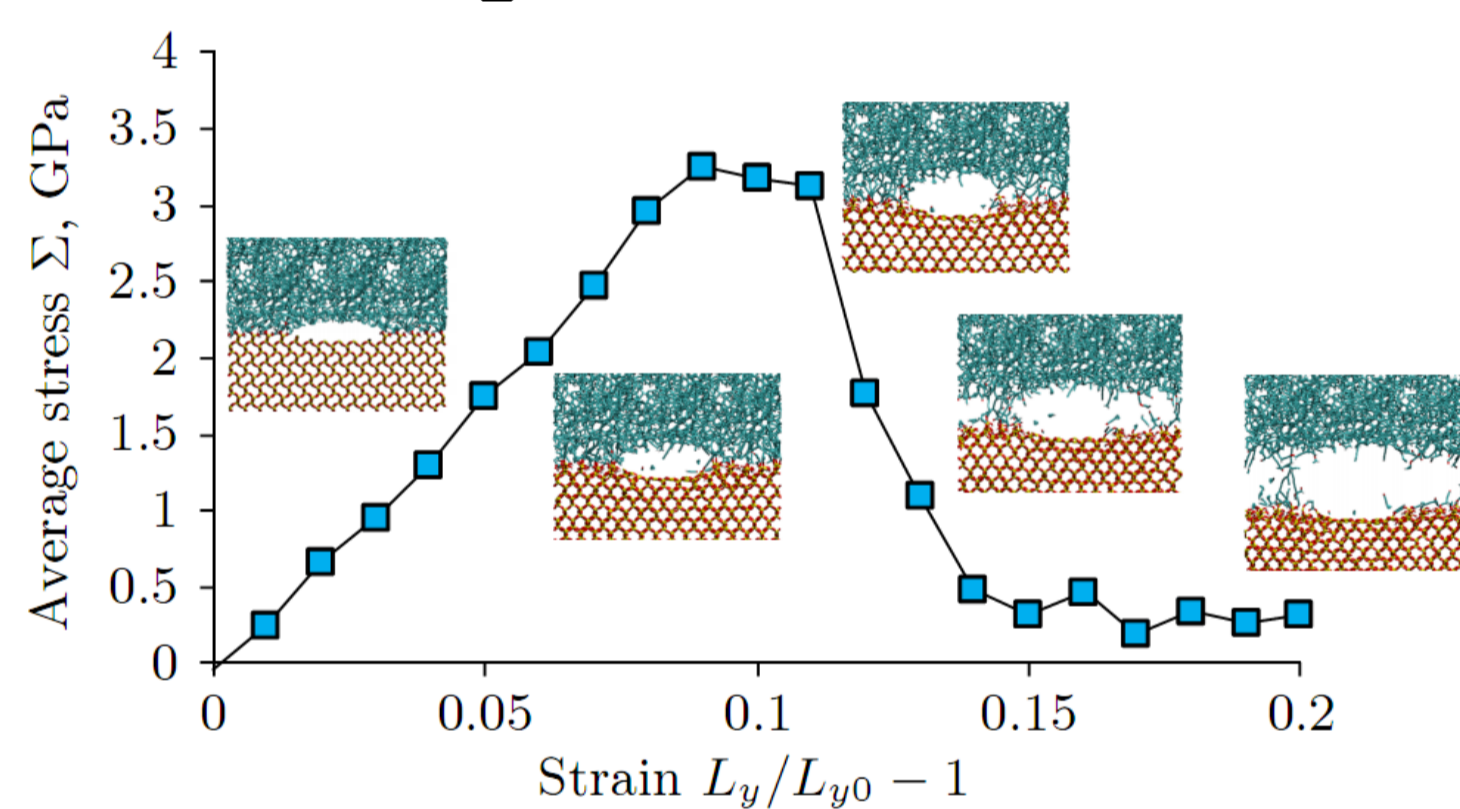


The loading curve of CS1000 shows a very progressive decrease, unlike silica, because of important irreversible atomic rearrangements at the crack tip.

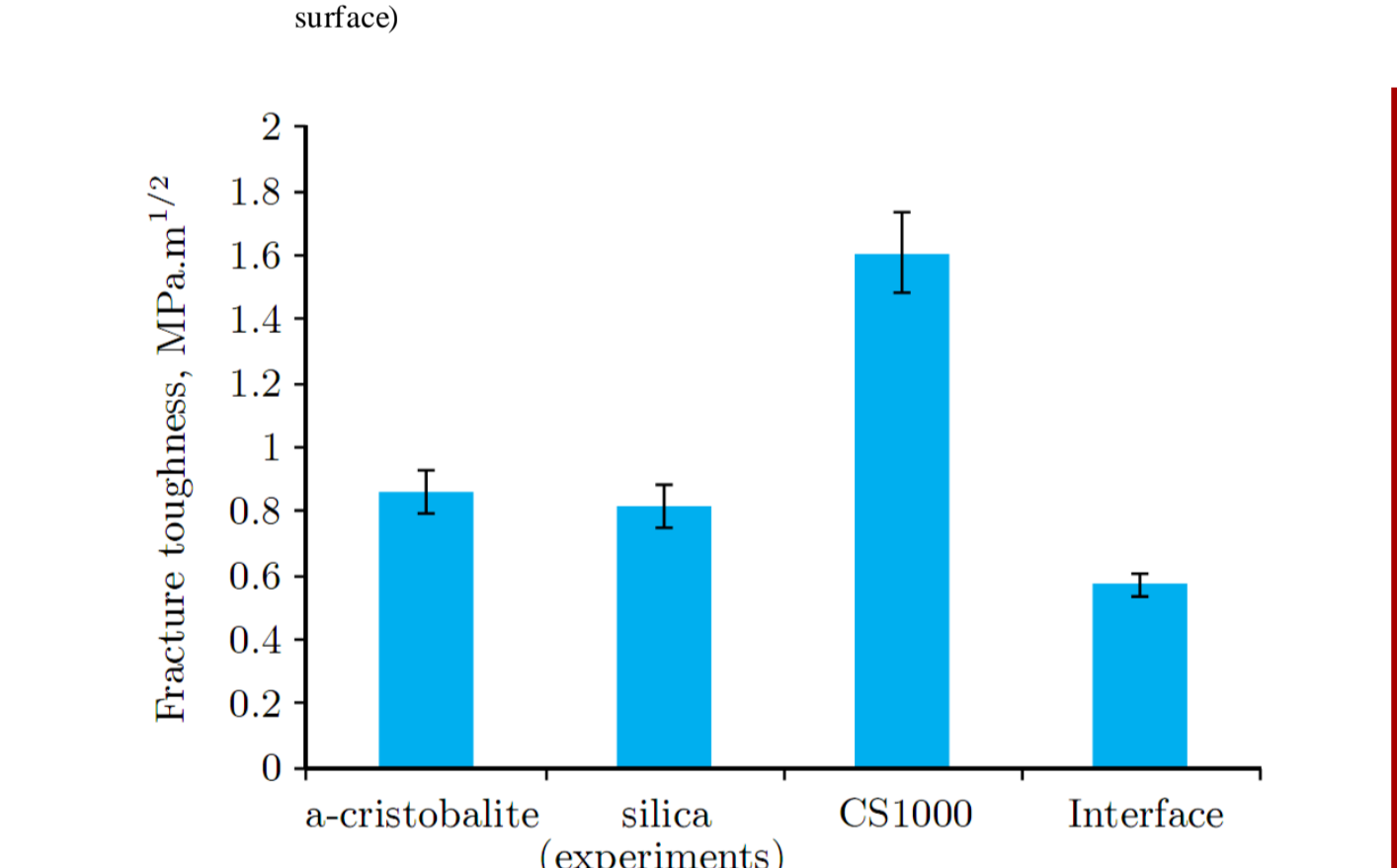
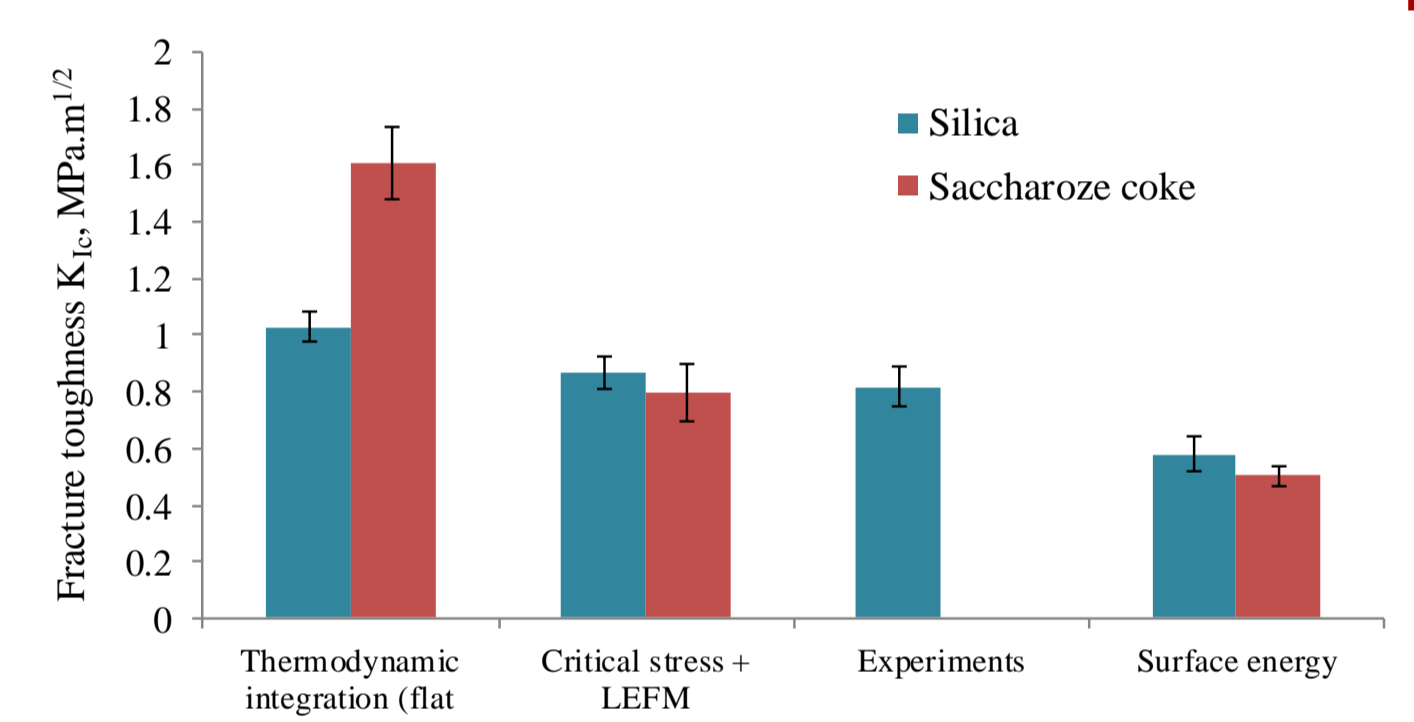
The toughness obtained by thermodynamic integration is two times larger than with LEFM. This proves the significant ductility of microporous carbons.



Silica-kerogen interface



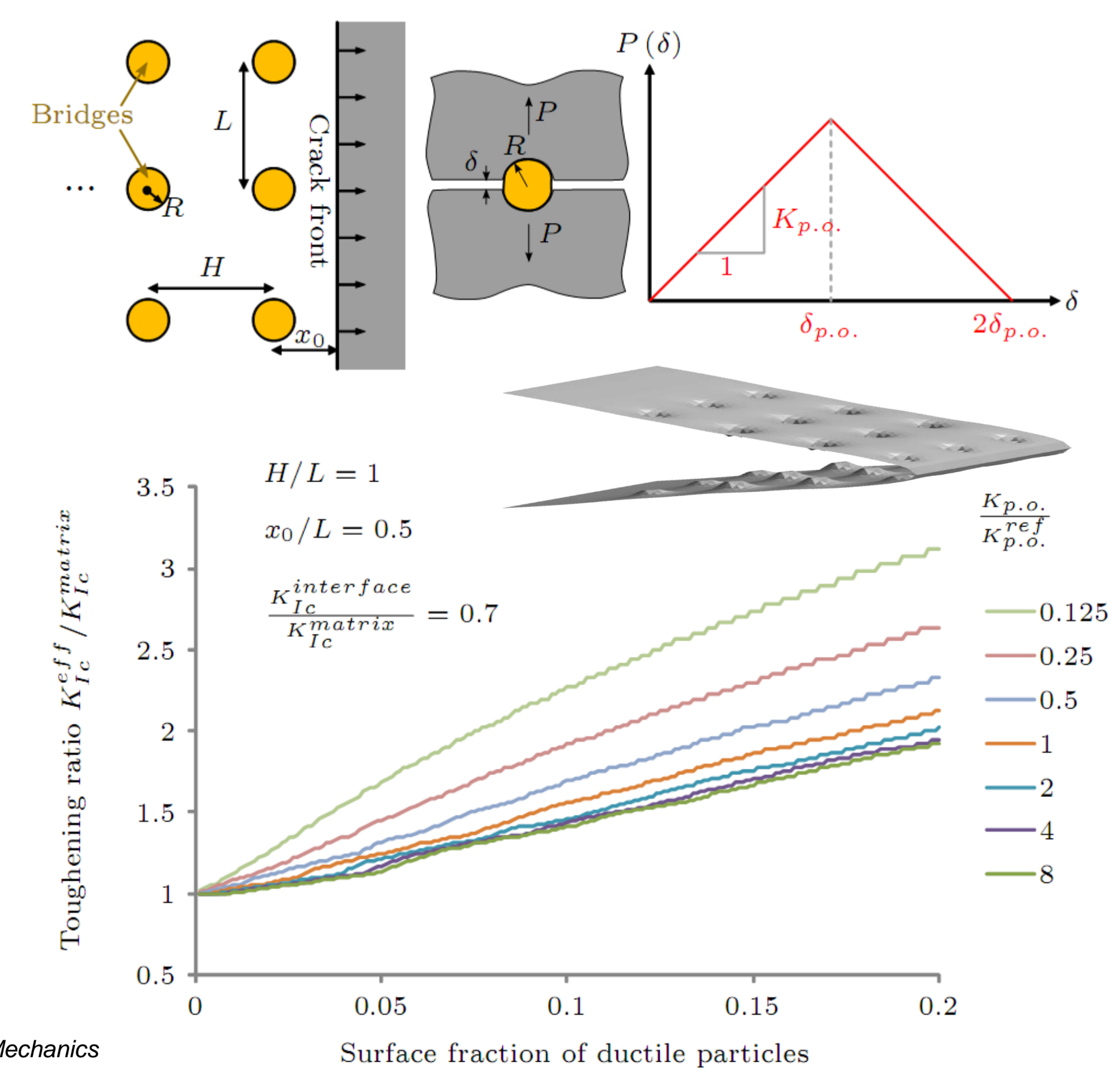
The silica-CS1000 interface also exhibits a significant ductility, although the absolute toughness is lower than that of the bulk phases



UPSCALING AT THE SCALE OF HETEROGENEOUS SHALE

We consider an up-scaling based on the particle pull-out phenomenon: ductile particle (kerogen/clay) in a brittle matrix (silica/carbonate) resist the opening of the crack. We use the numerical approach of Bower and Ortiz (1991) with a pull out law adapted to the case of shale.

⇒ Large toughening ratios even with small fractions of ductile inclusions



Numerical approach: Bower and Ortiz, *Journal of the Mechanics and Physics of Solids* (1991) 39:815

CONCLUSIONS

We propose a methodology to estimate fracture properties by molecular simulation. In particular, this methodology enables to identify the ductility of a material. We apply it to silica and kerogen, two of the main constituents of shale rocks. We validated the methodology by considering silica, which is a brittle linear elastic material, and for which experimental results are available in the literature. We identify an important ductility for bulk kerogen and kerogen-silica interface which is consistent with observation on shale rocks. Finally, we consider a up-scaling scenario to derive the fracture properties of heterogeneous shales, which shows that the ductility of shale can be very sensitive to a small amount of ductile inclusions like kerogen