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Thermo-mechanical influence on fracture propagation: integrating temperature effects through equilibrium statistical mechanics

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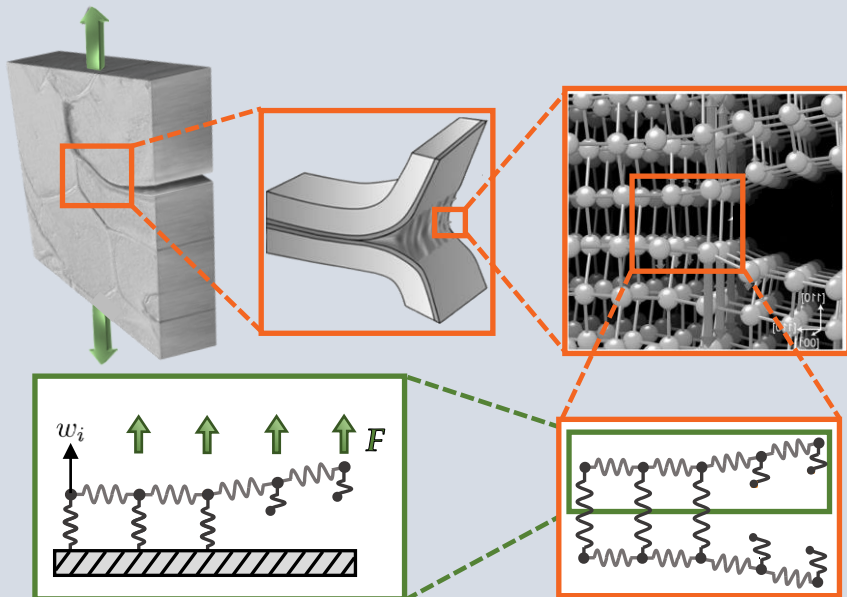


Introduction

This study addresses the thermal influence on fracture propagation in materials. Building upon the classical Griffith energy criterion for fracture, a simple model incorporating temperature effects is developed. By replacing the mechanical energy with thermodynamic quantities and using equilibrium statistical mechanics, it is possible to integrate entropic effects to explore how temperature influences fracture propagation.

A multiscale approach is employed, combining discrete and continuum models to account for temperature effects through statistical mechanics and provide a realistic description of the phenomenon. The developed model yields analytical results and reveals a critical temperature causing a spontaneous phase transition from intact to broken state even without an applied mechanical load.

Multiscale Approach

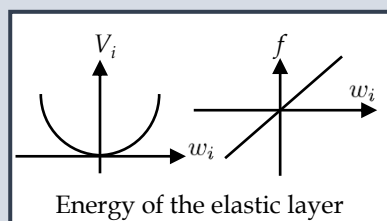
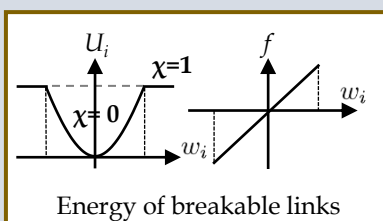


A **microscopic** model for fracture propagation has been formulated. The crack propagation is described by employing a **discrete** model made of a succession of n units. Each unit is modeled as an elastic spring and a breakable element that can switch from an attached to a detached state once the fracture threshold is reached.

We introduce an internal spin variable χ , which assumes value 0 when the breakable unit is intact and 1 when it is broken.

The spin variable allows us to write the total mechanical energy of the system in a more compact form:

$$g = \frac{1}{2}k_t \sum_{i=1}^n [(1 - \chi_i)w_i^2 + \chi_i] + \frac{1}{2}k_e \sum_{i=1}^{n-1} (w_{i+1} - w_i)^2 - \sum_{i=1}^n Fw_i$$



Equilibrium Solutions

The equilibrium configurations of the system are explored by means of **energy minimization**.

The **continuum limit** (number of units $\rightarrow \infty$, length of the system = fixed) is also evaluated, allowing for a more accurate comparison between the model and experimental results.

Classical Griffith energy criterion

We study a system with an initial crack ξ , and determine the critical value of the force required for crack propagation according to the classical Griffith's energy criterion.

$$\frac{\partial g_e}{\partial \xi} < 0 \rightarrow F > \frac{1}{1 + \frac{\xi}{\nu} \coth\left(\frac{1-\xi}{\nu}\right)}$$

Temperature effects

The thermal fluctuations in the system are introduced by means of classical **statistical mechanics** methods.

The partition function in the Gibbs ensemble reads:

$$\mathcal{Z}_G = \int_{\mathbf{R}^n} e^{-\frac{g}{k_B T}} dw_1 \dots dw_n$$

The Gibbs free energy of the system includes the entropic term

$$\mathcal{G} = H - TS = -k_B T \log \mathcal{Z}_G$$

The Griffith energy criterion for fracture propagation is extended to include the thermal effect by replacing the classical mechanical energy with the Gibbs free energy.

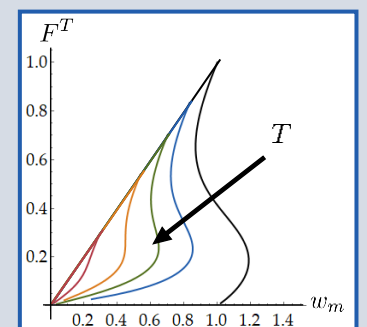
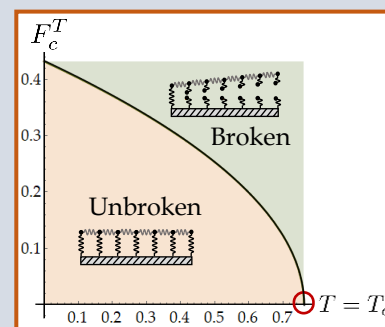
Results

The results indicate that the force required for fracture propagation is temperature dependent:

$$\frac{\partial \mathcal{G}}{\partial \xi} < 0 \rightarrow F^T > \frac{\sqrt{1 - \frac{T}{T_c}}}{1 + \frac{\xi}{\nu} \coth\left(\frac{1-\xi}{\nu}\right)}$$

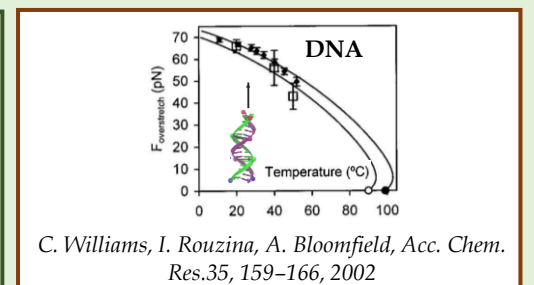
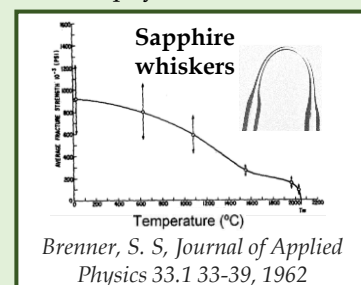
A critical temperature in correspondence of which the system undergoes a **phase transition** (spontaneous rupture) is determined

$$T_c = \frac{\nu E L b Y_m^2}{h k_B \coth\left(\frac{1-\xi}{\nu}\right)}$$



Conclusions

The **analytical** results obtained from the microscopic model reflect the phase transition behaviour observed **experimentally** in various systems ranging from biophysics to materials science.



Traditional fracture mechanics results (energy release rate, fracture toughness, and J-integral) are extended to incorporate temperature effects.

Some limitations of traditional fracture mechanics, such as stress singularity at the crack tip and fracture nucleation, are overcome.