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

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The study of the impact that thermal fluctuations have on fracture propagation represents an intriguing yet intricate subject, presenting both theoretical and experimental challenges across diverse scales of interest. Despite the plethora of experimental studies and numerical simulations analyzing the correlation between thermal fluctuations and mechanical properties, a notable absence of a robust theoretical framework in fracture mechanics that integrates temperature effects persists. In response to this gap, our study endeavors to elucidate the influence of temperature on material failure using the tools of equilibrium statistical mechanics. We employ a multi-scale approach to study how fracture propagation at the micro scale determines the macroscopic failure of the solid. Specifically we develop a discrete model that mimics crack propagation within a medium at the micro scale. This model consists of n successive units, each comprising an elastic spring (stiffness k_e) replicating the solid's elastic properties and a breakable unit (stiffness k_t) simulating fracture propagation. We underline that although the model is initially developed in the discrete form, mainly to account for the entropic effects, we also study the continuum limit (number of units of the system tending to infinity), which enables a more simple and compact analytical description of the physical phenomenon. We investigate the thermo-mechanical response of the system under a distributed force F, yielding a total mechanical energy expression

$$g = \frac{1}{2}k_t \sum_i (1-\chi_i)\, w_i^2 + \frac{1}{2}k_e \sum_i (w_{i+1}-w_i)^2 - F\sum_i w_i,$$

where, following the approach used in [1], we have introduced an internal spin variable χ_i which assumes value 0 when the link is intact and 1 when it is broken. After exploring the equilibrium configuration through energy minimization for a given crack length, we compute the stress required for fracture propagation, according to the traditional Griffith energy criterion [2]. The novelty in our model lies in extending this well-known criterion to incorporate thermal fluctuations. Thus, by employing equilibrium statistical mechanics, we integrate entropic effects into the overall energy balance. Specifically, we write the partition function in the Gibbs ensemble

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

which relate the mechanical energy of the system to a thermodynamic quantity, which is the Gibbs free energy

$$\mathcal{G} = H - TS = k_b T \ln \mathcal{Z}.$$

The crucial point of integrating thermal fluctuations into traditional fracture mechanics involves substituting the total mechanical energy with the Gibbs free energy. This approach enables us to derive fully analytical results describing the analytical dependence of the fracture threshold on temperature and, in particular, revealing the existence of a critical temperature, in correspondence of which the system undergoes a phase transition – the spontaneous rupture of the system without applying a mechanical load. This behavior reflects known experimental phenomena, including fracture in high and medium entropy alloys and nanowires, cell detachment, DNA and RNA denaturation.

References

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