LATTICE TRAPPING AND FRACTURE TOUGHESS SELECTION IN BRITTLE CRYSTALS

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Summary Predicting the resistance-to-failure from the solid structure at the atomistic scale remains unsolved, even in the simplest situations of perfectly brittle fracture. By examining numerically crack growth in electrical analogues of brittle crystals, we shed a new light on this question: Fracture toughness is found to be significantly higher than expected from Griffith's relationship between fracture and specific surface energy. This discrepancy finds its origin in the matching between the continuum displacement field at the engineering scale and the discrete lattice of solids at the atomic scale. We will show how to use the specific asymptotic form taken by this field near crack tip to infer this matching, and subsequently to predict toughness from the atomistic parameters. The implications will be discussed.

INTRODUCTION

Predicting when rupture occurs is central to many industrial, societal and geophysical fields. For brittle solids under tension, the problem reduces to the destabilization of a pre-existing crack. Material's resistance-to-failure is then defined by two dependent material constants (one is proportional to the square of the other): fracture energy and fracture toughness. Nowadays, there exists well-established standard test methods allowing the accurate experimental determination of these material constants. Conversely, their relation with the atomistic parameters of the considered solid remains unsolved, even in perfectly brittle situations where fracture occurs via successive bond breaking, without involving further elements of dissipation. The cornerstone in this context was provided by Griffith [1], which identifies the fracture energy with the free surface energy (energy of the chemical bonds crossed by a fracture surface of unit area). Unfortunately, this conjecture does not fit with the observations: Fracture energy is always measured to be anomalously high, even in perfectly brittle crystals (silicon or mica for instance, see. e.g. [2]). The study reported here aimed at uncovering the origin of this discrepancy.

METHOD & RESULTS TO BE PRESENTED

We examined numerically how crack propagates in a two-dimensional lattice of fuses arranged periodically (triangular, square or honeycomb geometry, see e.g. figure 1A). Such model digital materials, indeed, (i) possess fully prescribed and tuneable "atomic bonds"; (ii) break in a perfectly brittle manner, by the successive breakdown of fuses, and (iii) satisfy isotropic linear elasticity under antiplane deformation at the continuum scale [3]. Fracture energy was determined in these digital materials and, as in real elastic solids, it was found to be significantly larger than Griffith specific surface energy, by a factor depending on the lattice geometry.

To understand the origin of this discrepancy, we looked at the spatial distribution of the displacements within the digital materials (Figure 1B). At the continuum-level scale, the displacement field displays a mathematical singularity at the crack tip. As such, it takes a generic asymptotic form [4], referred to as Williams' series expansion. The difficulty is to position the singularity origin properly in the discrete lattice at the atomic scale. As an illustration, placing it at the center of the next bond to break (O_{guess} in figure 1A) makes the Williams's series expansion describe the measured field fairly well, except in the very vicinity of the crack tip [figure 1C]. Unfortunately, this near-tip zone is precisely the one setting whether or not the next bond breaks!

However, as we will see in the presentation, it is possible to make use of the Williams' form taken by the displacement field near crack tip to infer accurately the singularity positioning in the discrete lattice, and then to predict fracture toughness from the atomistic parameters [5]. It is then possible to derive an analytical method to predict fracture toughness and fracture energy in our digital materials and the obtained values coincide exactly to those obtained numerically. We will discuss how to extend the analysis to genuine elastic (plane stress) crack problems and predict toughness in 2D and 3D materials. Implication will be finally discussed.

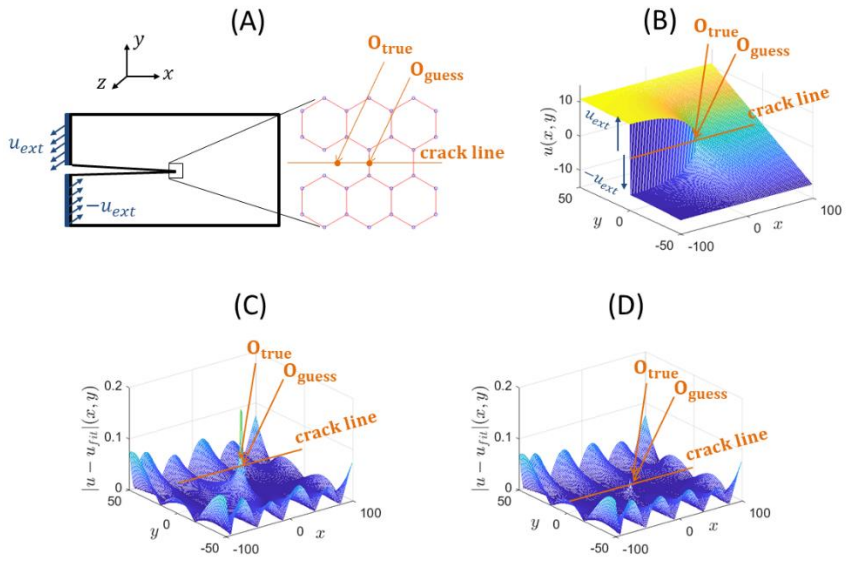

Figure 1, panel A: Sketch and notation: A crack is introduced into a two-dimensional electric crystal (here honeycomb lattice). The crack is parallel to x-axis, lies in the middle of the crystal ($y = 0$) and stops in the center. The cracked crystal is loaded by imposing a constant potential u_{ext} (opposite signs) to the left/ top and left/bottom edges. Panel B: measured displacement field. This should obey Williams asymptotic singular form. The difficulty is to place the singularity properly in the discrete lattice. Panel C: Absolute difference between the displacement field $u(x,y)$ measured in panel B and Williams asymptotic form, $u_{fit}(x,y)$ obtained after having placed the singularity at the center of the next bond to break (O_{guess} in panel A). The fit is very good everywhere, except in the vicinity of the crack tip. Panel D: $|u_{fit} - u(x,y)|$ after having corrected the singularity position (now at O_{true} in panel A). The fit is now good everywhere, including in the very vicinity of the crack tip.

References

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