Cross-scale description of crack propagation in few-layer graphene stacks

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Fracture of carbon fibers is a complex multi-scale problem, which depends on the atomistic structure of individual carbon layers but also on the presence of pores and cracks on the microscopic scale. Here, we propose a combination of a continuum phase-field model with a molecular dynamics simulation to describe crack propagation in few layer graphene stacks. Different from a discrete crack representation, phase-field models solve an additional scalar field problem representing the regularised crack topology. The so-called phase-field is coupled to the mechanical boundary value problem. Cumbersome topological updates of the analysis mesh are avoided. Phase-field models for brittle fracture [1] allow for the proper modelling of crack initiation and propagation.

In this work, molecular dynamics (MD) simulations are used for the identification of additional material parameters introduced by the crack regularisation. On the atomic scale, cracks are propagated in single layer and few layer graphene (see Fig. 1). Due to the microscopic structure, the crack is not straight anymore but propagates along a wavy path. As in [2], the waviness alters the critical fracture energy at which the crack propagates. The MD results are used to obtain a macroscopic straight crack path in the phase-field simulation with the same critical value for crack propagation (see Fig. 2). The combination of MD and phase-field simulations allows it to study the influence of atomistic defects on macroscopic mechanical properties, such as the fracture toughness, of the macroscopic system.

References

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[2] M. Hossain, C.-J. Hsueh, B. Bourdin, K. Bhattacharya, *Journal of the Mechanics and Physics of Solids* 71 (2014) 15-32.

Figures

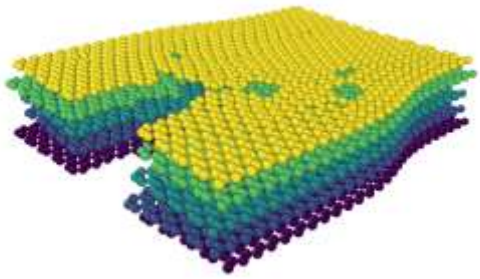

Figure 1: Five-layer graphene stack after initial rupture calculated using a classical molecular dynamics simulation.

Figure 2: Crack propagation obtained from a phase-field simulation assuming a homogeneous material.