ATOMISTIC MODELLING OF MATERIALS (MT41028)

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MD simulations of uniaxial deformation of a monolayer graphene

Question1: (a) The fracture stress (σ_f) depends on inherent flaw size. Use the following input files (i) longcrack.in, (ii) mediumcrack.in, and (iii) shortcrack.in to evaluate the effect of *initial crack length* on the fracture stress of monolayer graphene at 300 K. (2 credit). You can use Ovito to calculate initial crack length for all the inputs files (see the attached video).

(b) Using Ovito, show σ_{YY} contour of the samples at the onset of crack initiation. What do you see at the crack tip in terms of the magnitude of stress. (1.5 credit)

Question2: Fracture toughness (G_c) is a fundamental property which determines any materials ability to resist crack propagation. The fracture toughness of graphene under plane stress condition can be calculated, assuming linear elastic fracture mechanics. The expression for G_C is:

$$G_c = \frac{\pi \sigma_f^2 a}{E} \tag{1}$$

where, a is the half crack length (for clarity, see the illustration below (Fig. 1)) and E is the Young's modulus. You have already calculated the Young's modulus of pristine graphene during the lab session. Using Eq. (1), calculate the value of G_c for graphene at 50 K, 300 K, 500 K in units of J/m^2. Does G_C depend on crack length and temperature? (2.5 credit)

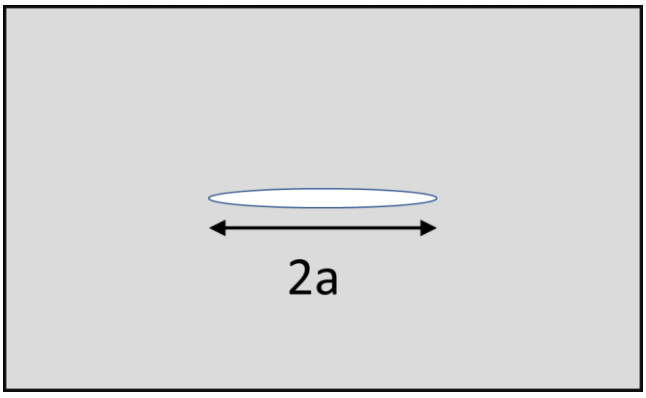

Figure 1: Illustration of crack length (2a)