Elasticity and fracture: Is there a connection?

Petr Lazar, Raimund Podloucky and Walter Wolf

Center for
Computational Materials Science

Mechanical properties of material

Elasticity: determines response of material subjected to small strains; related physical quantities are elastic constants

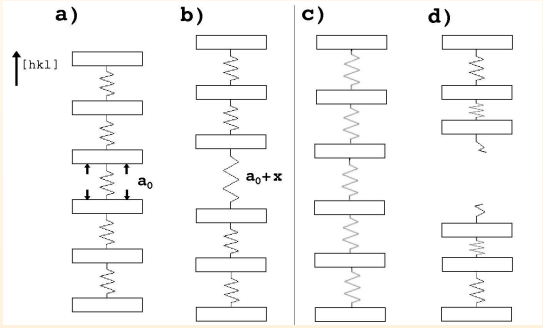
Fracture: describes nucleation and propagation of cracks.

- propagating crack lead to sudden failure of material - important for engineering applications
- the processes which contribute to crack energy span over several length scales - a description within one general theory impossible

Crack at atomic level

at atomic level crack propagates by consequent breaking of atomic bonds; cleavage decohesion of atoms in crystal

cleavage can be modeled via DFT method



For rigid block separation the energy is a function of x (UBER): [1]

$$E_{DFT}(x) = G_b \left[\left(1 + \frac{x}{l_b} \right) \exp\left(-\frac{x}{l_b} \right) - 1 \right]$$

G_b ..... cleavage energy
l_b ..... critical length

Stress $\sigma(x) = \frac{dE}{dx}$

Critical stress $\sigma_b = \max \sigma(x) = \sigma(x = l_b)$

$$\sigma_b = \frac{1}{e} \frac{G_b}{l_b}$$

[1] Rose et al. *Phys. Rev.* B 28 (1983)