Elasticity and fracture: a connection

Petr Lazar, Raimund Podloucky and Walter Wolf

Center for
Computational Materials Science
http://www.cms.tuwien.ac.at

ELASTICITY: determines response of material subjected to small strains; related physical quantities are elastic constants - easy to measure or calculate

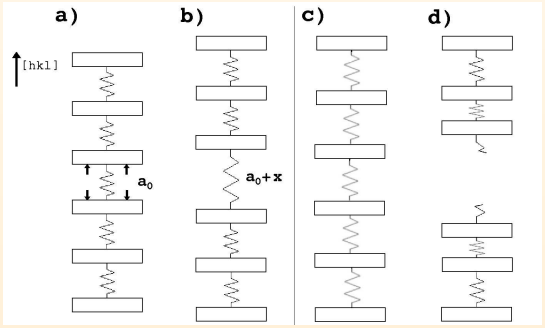
FRACTURE: describes nucleation and propagation of cracks.

- propagation of 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
- brittle fracture: no plastic dissipative processes during crack propagation, technologically important

direct ab initio modelling of crack impossible

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

cleavage decohesion can be modeled via DFT method:



Ideal Brittle Cleavage

NO atomic RELAXATION when material is cleaved:
very FAST crack formation
UPPER limit of strength for ideal brittle materials

+ analytic model for crack formation

+ analytic model for
  CONNECTION ELASTICITY - CRACK FORMATION

+ model parameters determined by fit to DFT calculations [1]

[1] VASP, G. Kresse et al., CMS and Univ. Vienna

For rigid block separation the energy is a function of x (UBER): [2]

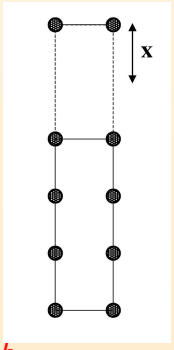
$$E_{DFT}(x) = G_b \left[\left(1 + \frac{x}{l_b} \right) \exp \left(-\frac{x}{l_b} \right) - 1 \right]$$

G_b ..... cleavage energy

l_b ..... critical length

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

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



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

[2] Rose et al. *Phys. Rev.* B 28:1835 (1983)

Earlier estimates of theoretical cleavage stress

1. Orowan's criterion:[3][4] assumption of sinusoidal variation of restraining force

$$\sigma_{max} = \sqrt{\frac{E\gamma_s}{a_0}}$$

E...Young's modulus
γ_s...surface energy
a_0...distance between layers

2. Orowan's criterion often overestimates theoretical cleavage stress

3. fit to ab-initio calculations[5]: model not reliable

[3] M. Polanyi, Z. Phys 7:323 (1921)
[4] E. Orowan, Rep. Prog. Phys. 12:185 (1949)
[5] M. H. Yoo and C. L. Fu, Mat. Sci. Eng, A153:470 (1992)

Connecting elasticity and fracture - assumptions:

A very small crack-like preturbation may develop into:

- the crack - the energy is localised in a local volume V_{loc} around crack
- elastic response - the energy is spread over the volume of material

unstable equilibrium between cleavage crack formation and elastic response

under plane stress conditions (our cleavage model) $V_{loc} = AL_b$

A...crack area

L_b...localisation length (fit parameter)

BRITTLE: Crack remains open for any $x > 0$. At $x \approx 0$

$$\frac{1}{2} A G_b \frac{x^2}{l_b^2} = \frac{1}{2} A L_b c'_{11} \frac{x^2}{L_b^2}$$

Left side: Taylor expansion of UBER in second order of x.
Right side: elastic energy according to the elastic modulus c'_{11} localised in volume $V = AL_b$ with L_b the brittle localisation length.

Then we derive:

$$L_b = c'_{11} \frac{l_b^2}{G_b}$$

$$\sigma_b = \frac{1}{e} \sqrt{\frac{G_b c'_{11}}{L_b}}$$

Fe, Al, W: important structural materials

brittle transition at low temperatures

	$[hkl]$	c_{11}	G_b/A	l_b	σ_b/A	a_0	L_b
Al (fcc)	100	110	1.8	0.57	12	2.03	2.01
	110	113	2.1	0.64	12	1.43	2.24
	111	114	1.6	0.54	11	2.34	2.08
Fe (bcc)	100	302	5.3	0.58	34	1.41	1.93
	110	338	5.0	0.54	35	1.99	1.97
	111	350	5.8	0.61	35	0.82	2.25
W (bcc)	100	540	8.4	0.66	47	1.59	2.80
	110	516	6.5	0.55	44	2.24	2.40
	111	508	7.3	0.64	42	0.92	2.83

perspective high-strength high-temperature materials; turn brittle at ambient temperatures

		$[hkl]$	c_{11}	G_b/A	l_b	σ_b/A	a_0	L_b
NiAl	B2	100	203	4.8	0.69	26	1.45	2.01
		110	284	3.2	0.54	22	2.05	2.59
		111	311	4.1	0.58	26	0.84	2.68
		211	284	4.0	0.60	24	1.18	2.56
Ni_3Al	$L1_2$	100	225	4.3	0.66	24	1.78	2.28
		111	331	3.7	0.52	26	2.06	2.42
FeAl	B2	100	278	4.8	0.71	25	1.43	2.92
		110	354	4.3	0.50	32	2.03	2.06
		111	380	5.1	0.61	31	0.83	2.77
Al_3Sc	$L1_2$	100	189	2.7	0.61	16	2.05	2.60
		110	182	2.9	0.65	17	1.45	2.65
		111	180	2.6	0.61	16	2.37	2.58
TiAl	$L1_0$	001	185	4.4	0.70	23	2.03	2.06
		100	190	3.3	0.58	21	2.00	1.98
		110	240	4.1	0.69	22	1.41	2.82
		111	268	3.5	0.58	22	2.32	2.57

trasition metal carbides: hard but brittle materials, strong covalent bonding

MgO is important ceramic material

		$[hkl]$	c_{11}	G_b/A	l	σ_b/A	a_0	L_b
VC	B1	100	647	3.2	0.37	32	2.08	2.77
		110	585	7.0	0.55	46	1.47	2.53
		111	564	9.9	0.58	63	1.20	2.06
TiC	B1	100	515	3.5	0.42	31	2.17	2.57
		110	489	7.7	0.56	51	1.53	1.97
		111	481	11.6	0.70	61	1.25	2.03
MgO	B1	100	299	1.8	0.37	18	2.11	2.27
		110	345	4.4	0.54	30	1.53	2.29
NaCl	B1	100	52	0.3	0.49	2	2.83	4.16
		110	45	0.7	0.66	4	2.00	2.84

Conclusions

+ Utilising the idea of localisation of elastic energy, the connection between elasticity and cleavage is established via introduction of a new materials quantity called localisation length L_b.

+ By combining *ab initio* results and analytic models the parameter L_b is determined. For brittle cleavage it is rather constant, $L_b \approx 2.4$ Å, for all (studied) materials and directions.

+ Model tested for different types of bonding (metallic, ionic, covalent).

+ Similar connection between elasticity and cleavage can by established for case of relaxed cleavage - Lazar, Podloucky, Wolf: *submitted to* PRB