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Elasticity and fracture: Is there a connection?

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Estimates of theoretical cleavage stress

1. Orowan's criterion:[1,2] 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[3]: model not reliable

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[1] M. Polanyi, Z. Phys 7, (1921)
[2] E. Orowan, Rep. Prog. Phys. **12** (1949)
[3] M. H. Yoo and C. L. Fu, Mat. Sci. Eng, **A153** (1992)

Crack model:

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For rigid block separation the energy is a function of x (UBER): [4]

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

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

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

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

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

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

Atoms are allowed to relax after initial crack: either the crack disappears (elastic response) or the material broken and relaxed surfaces are created.

At the critical point l_e elastic energy is localized within t

$$G_e = \frac{1}{2} A c'_{11} \frac{l_e}{L_e}$$

Elastic energy

$$E(x) = \frac{G_e}{l_e^2} x^2$$

Maximum of the stress in the elastic limit

$$\sigma_e = 2\frac{G_e}{l_e}.$$

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Connecting elasticity and fracture - key assumptions:

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:

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

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

ELASTIC: Crack opens for $x > l_e$. At the critical crack size $x = l_e$ the elastic energy $E_e(l_e) = G_e$ is equal to the cleavage energy.

$$G_e = \frac{1}{2} A L_e c'_{11} \frac{l_e^2}{L_e^2}.$$

Elastic energy localised in volume AL_e with L_e the elastic localisation length.

$$L_e = \frac{1}{2} \frac{c'_{11} l_e^2}{G_e}$$

$$\sigma_e = \sqrt{\frac{2 G_e c'_{11}}{L_e}}$$

For elastic cleavage energy is a quadratic function of x

$$E_{DFT}(x) = G_e \frac{x^2}{l_e^2}$$

G_e ..... relaxed cleavage energy
l_e .... critical length

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

Critical stress $\sigma_e = \max \sigma(x) = \sigma(x = l_e)$

$$\sigma_e = 2 \frac{G_e}{l_e}$$

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

Critical stress: $\max \sigma(x) = \sigma(x = l_b) = \frac{G_b}{el_b}$

With connection established:

$$\sigma_b = \frac{1}{e}\sqrt{\frac{G_b c_{11}}{L_b}}$$

Calculated values - brittle limit

	$[hkl]$	a_0 Å	l_b Å	L_b Å	l_e Å	L_e Å
NiAl	001	1.45	0.69	2.0	2.7	15.8
	011	2.05	0.54	2.5	2.0	17.7
	111	0.84	0.58	2.4	2.2	18.4
TiAl	001	2.03	0.82	2.6	3.0	17.5
VC	001	2.16	0.37	2.8	0.8	6.5
MgO	001	2.11	0.37	2.2	0.8	5.3
TiC	001	2.17	0.42	2.6	1.3	11.9

	$[hkl]$	c'_{11} GPa	G_b J/m^2	σ_b GPa	G_e J/m^2	σ_e GPa
NiAl	001	203	4.8	26	4.6	34
	011	284	3.2	22	3.1	32
	111	327	4.1	26	3.9	36
TiAl	001	168	4.4	20	4.2	28
VC	001	647	3.2	32	2.4	60
MgO	001	299	1.8	18	1.7	42
TiC	001	515	3.5	31	3.2	50

Calculated values - brittle limit

	direction $[hkl]$	c'_{11} GPa	G_b J/m^2	l_b Å	σ_b GPa	L_b Å
NiAl	001	203	4.8	0.69	26	2.0
	011	284	3.2	0.54	22	2.5
	111	327	4.1	0.58	26	2.4
TiAl	001	168	4.4	0.82	20	2.6
	111	262	3.5	0.58	22	2.6
VC	001	647	3.2	0.37	32	2.8
	011	585	7.0	0.55	46	2.5
	111	564	9.9	0.58	63	1.9
Fe	001	302	5.4	0.59	34	2.0
	111	350	5.8	0.61	35	2.3
MgO	001	299	1.8	0.37	18	2.2
	011	345	4.4	0.54	30	2.3

Elastic limit

	direction [hkl]	G_e (J/m^2)	l_e (Å)	L_e (Å)	σ_e (GPa)
NiAl	100	4.6	2.7	15.8	34
	110	3.1	2.0	17.7	32
	111	3.9	2.2	18.4	36
TiAl	001	4.2	3.0	17.5	28
MgO	001	1.7	0.8	5.3	42
VC	001	2.4	0.8	6.5	60
TiC	001	3.2	1.3	11.9	50

Localisation lenghts in both limits

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Correlation between critical lengths in both limits

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Conclusions

+ Studying crack mode I the two limiting cases, BRITTLE and ELASTIC cleavage, can be described reasonably well by analytic models in comparison to *ab initio* DFT results.

+ The connection between elasticity and cleavage is established by a localisation length L.

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

+ Models and derivations valid for different types of bonding (metallic, ionic, covalent).

+ Similar (but more complicated) connections between elasticity and cleavage for crack modes II and III might be established on the same concept of localisation of elastic energy (or delocalisation of cleavage energy).

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