Elasticity and fracture: Is there a connection?

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Estimates of theoretical cleavage stress

1. Orowan's criterion:[1 2] Orowan assumed sinusoidal variation of restraining force $\sigma = K \sin \frac{\pi}{a}(x - a_0)$ and found constants K and a by setting $\int_{a_0}^{a_0+a} \sigma dx = 2\gamma_s$ and relating initial slope of σ to Young's modulus E. Then

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

2. Orowan's formula overestimate theoretical cleavage stress, however attempts to relate σ_{max} to other macroscopic physical properties still led to a higher estimates[3]

3. application of Orowan's criterion in ab-initio calculations and comparison with exact cleavage stress were made by Yoo and Fu[4]

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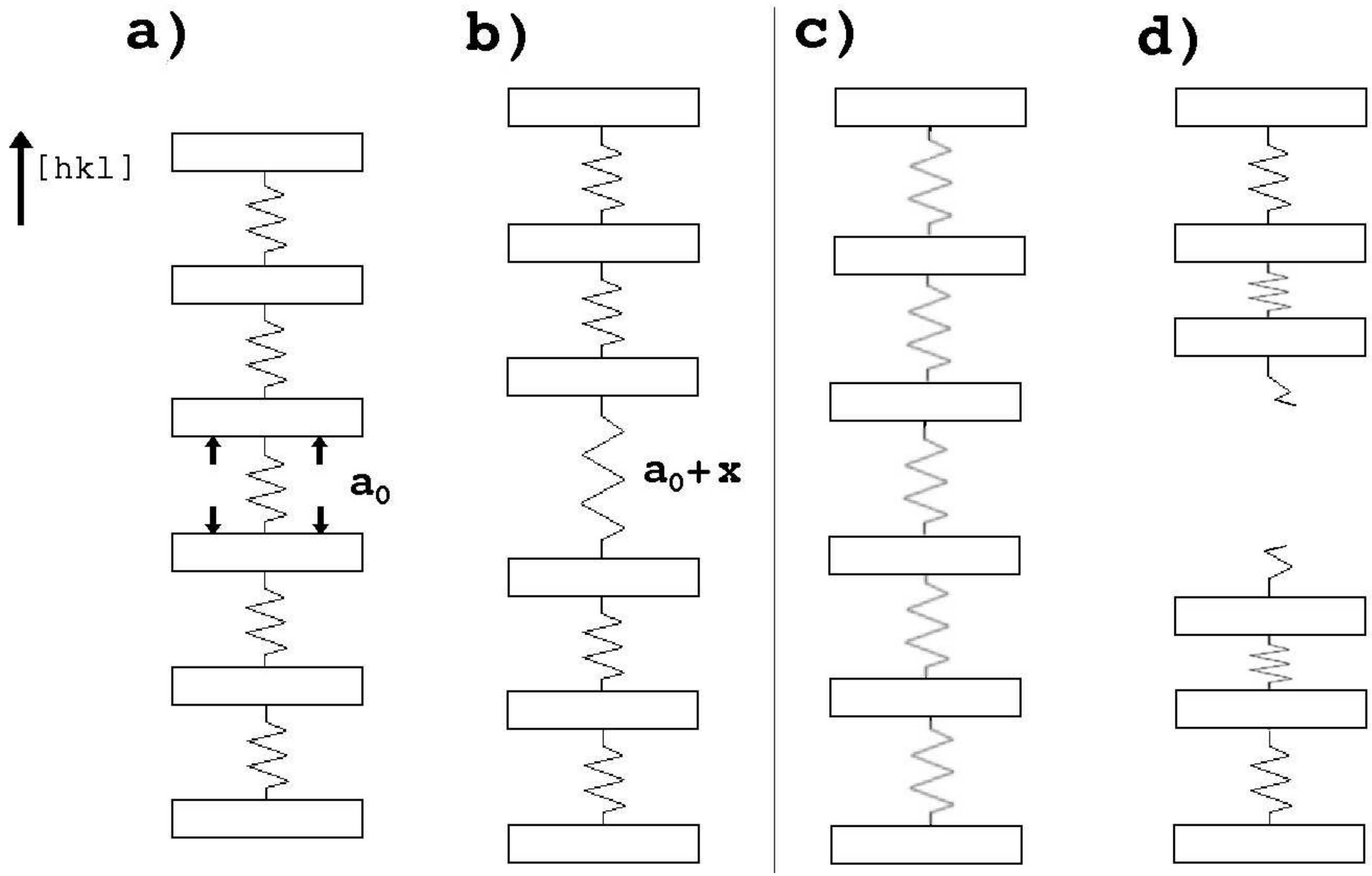
[1] M. Polanyi, Z. Phys **7**, (1921)
[2] E. Orowan, Rep. Prog. Phys. **12** (1949)
[3] J. J. Gilman, The strength of ceramic solids (Gordon & Breach, New York, 1963)
[4] M. H. Yoo and C. L. Fu, Mat. Sci. Eng, **A153** (1992)

Crack model:



For rigid block separation energy scales with x as[5]

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

Fitting this relation (called UBER) to calculated energies, cleavage energy G_b and critical length l_b (a length where material breaks) could be determined.

The stress $\sigma(x) = \frac{dE}{dx}$ reaches its maximum at $x = l_b$ and it amounts to

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

The critical lenght l_b depend on actual shape of interatomic forces and therefore is NOT accesible to experiments!

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

When atoms are allowed to relax, they close initial crack and respond elastically until a relaxed value of cleavage energy G_e is reached - at this is critical point l_e the crack is opened.
Therefore we can put

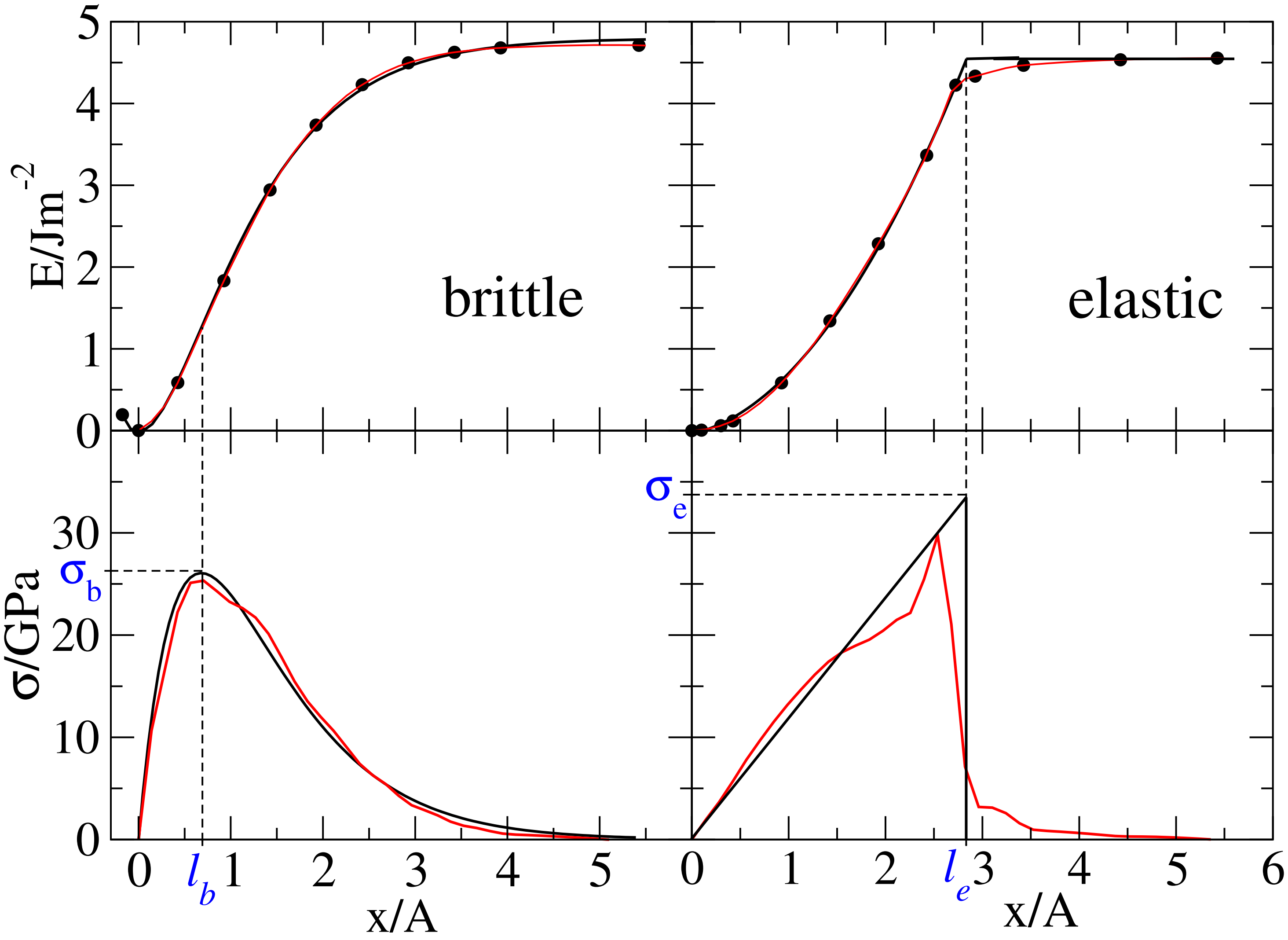
$$G_e = \frac{1}{2} A c_{11} \frac{l_e}{L}$$

and get

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

Maximum of the stress in the elastic limit is then

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



E/Jm^-2
σ/GPa
brittle
elastic
σ_b
σ_e
l_b
l_e
x/A
x/A

Connecting elasticity and fracture - key assumptions:

Assumption 1: at the critical limit $x = l_b$ (the crack just forms) elastic energy and cleavage are at an unstable equilibrium, the elastic energy is localised in a local volume $V = AL_b$.

$$L_b = c_{11}\frac{l_b^2}{G_b}$$

As a fitting result: L_b is rather constant, independent of material and direction!!!

Assumption 2: 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 lowest (second order) of x. Right side: elastic energy in volume $V = AL_b$ described by elastic modulus c'_{11}[6]

[6] $c'_{11}[hkl] = c_{11} - 2(c_{11} - c_{12} - 2\, c_{44})(h^2k^2 + k^2l^2 + l^2h^2)$

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

	direction $[hkl]$	c'_{11} GPa	G_b J/m^2	l_b $\AA$	σ_b GPa	L_b $\AA$	G_e (J/m^2)	l_e ($\AA$)	σ_e (GPa)	L_e $\AA$)
NiAl	001	203	4.8	0.69	26	2.0	4.6	2.7	34	15.8
	011	284	3.2	0.54	22	2.5	3.1	2.0	32	17.7
	111	327	4.1	0.58	26	2.4	3.9	2.2	36	18.4
TiAl	001	168	4.4	0.82	20	2.6	4.2	3.0	28	17.5
VC	001	647	3.2	0.37	32	2.8	2.4	0.8	60	6.5
MgO	001	299	1.8	0.37	18	2.2	1.7	0.8	42	5.3
TiC	001	515	3.5	0.42	31	2.6	3.2	1.3	50	11.9

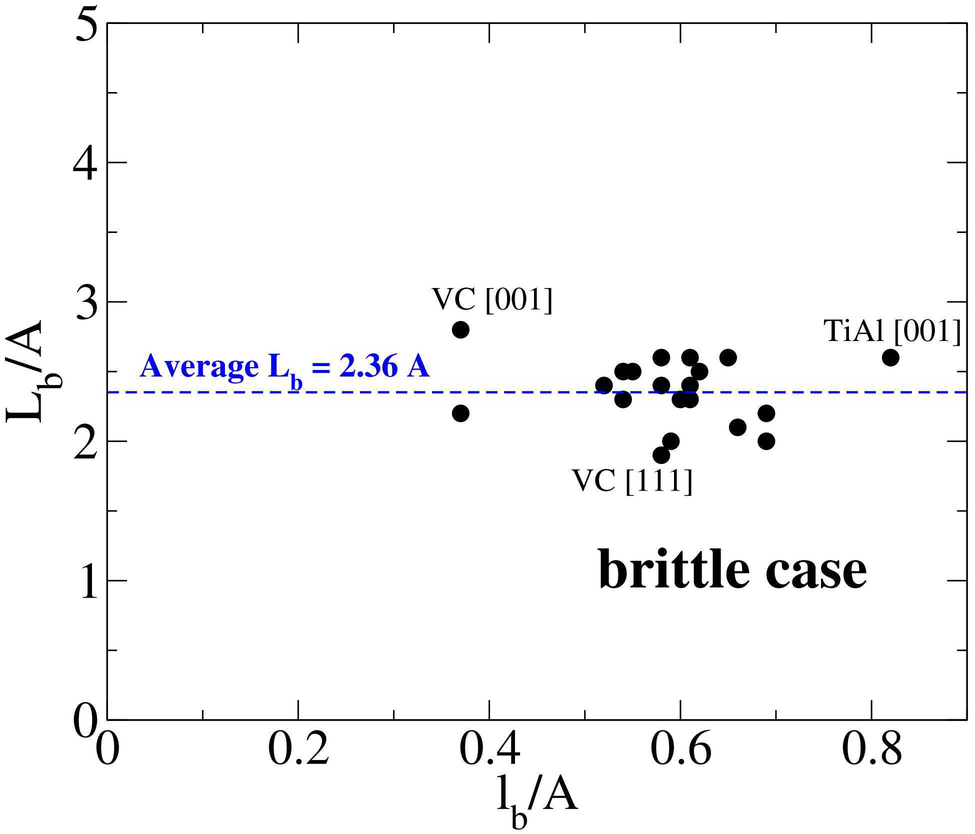
Calculated values - brittle limit

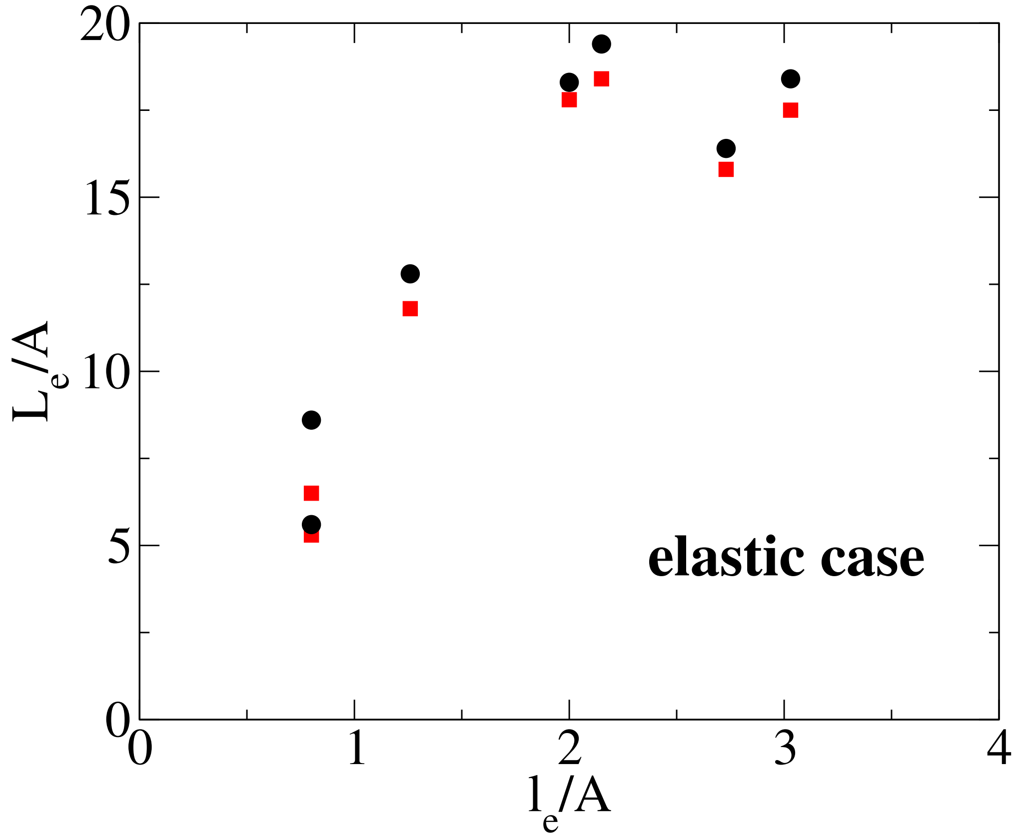
	direction $[hkl]$	c'_{11} GPa	G_b J/m^2	l_b Å	σ_b GPa	L_b Å
NiAl	001	203	4.8	0.69	26	**2.0**
	011	284	3.2	0.54	22	**2.5**
	111	327	4.1	0.58	26	**2.4**
Al_3Sc	001	189	2.7	0.61	16	**2.6**
	011	182	2.9	0.65	17	**2.6**
	111	180	2.6	0.61	16	**2.4**
TiAl	001	168	4.4	0.82	20	**2.6**
	111	262	3.5	0.58	22	**2.6**
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

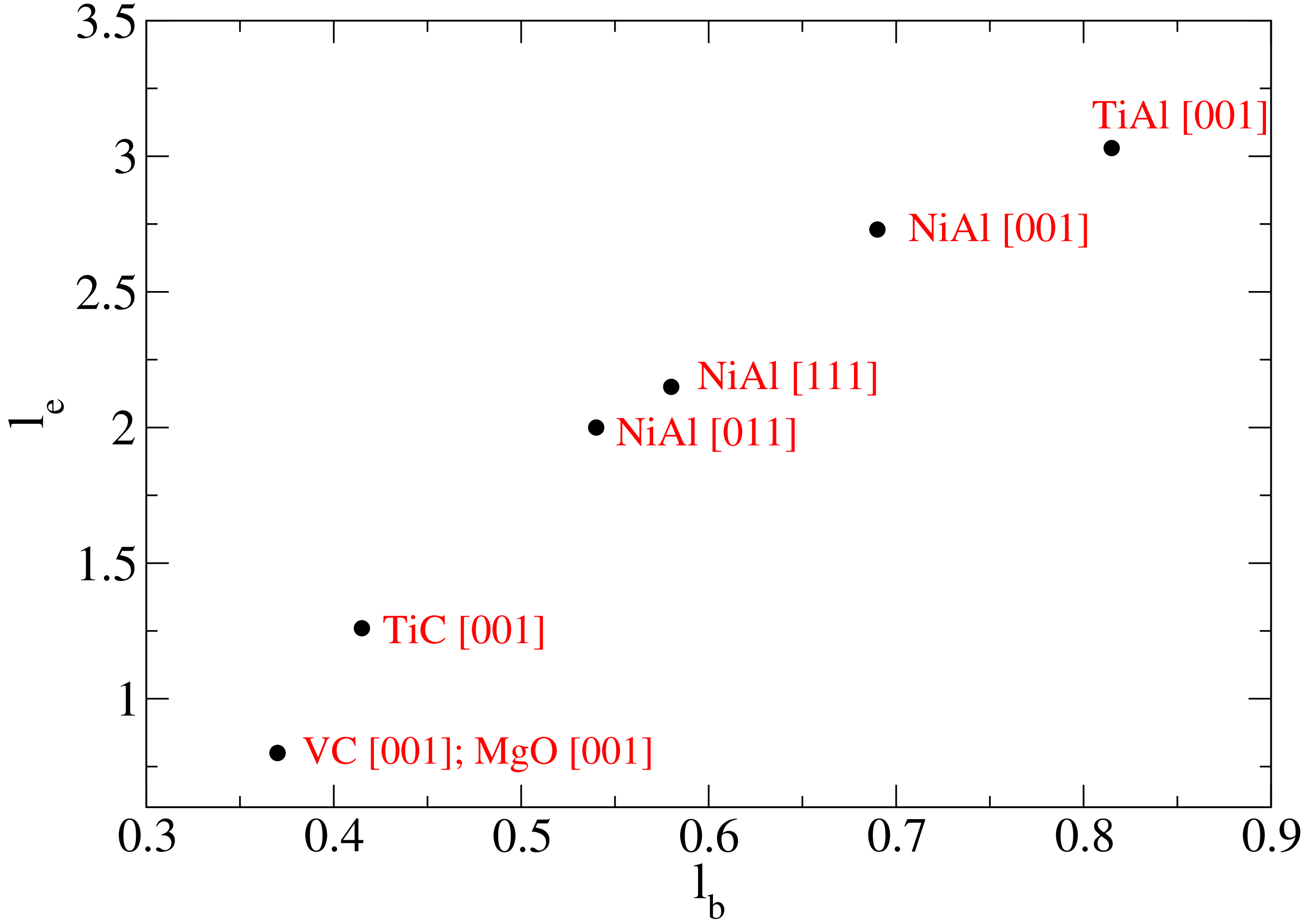
	direction $[hkl]$	G_e (J/m^2)	l_e ($\AA$)	L_e ($\AA$)	σ_e (GPa)
NiAl	100	4.6	2.7	15.8	34
	110	3.1	2.0	17.7	32
	111	3.9	2.2	18.4	36
TiAl	001	4.2	3.0	17.5	28
MgO	001	1.7	0.8	5.3	42
VC	001	2.4	0.8	6.5	60
TiC	001	3.2	1.3	11.9	50

Localisation lenghts in both limits





Correlation between critical lengths in both limits



Conclusions

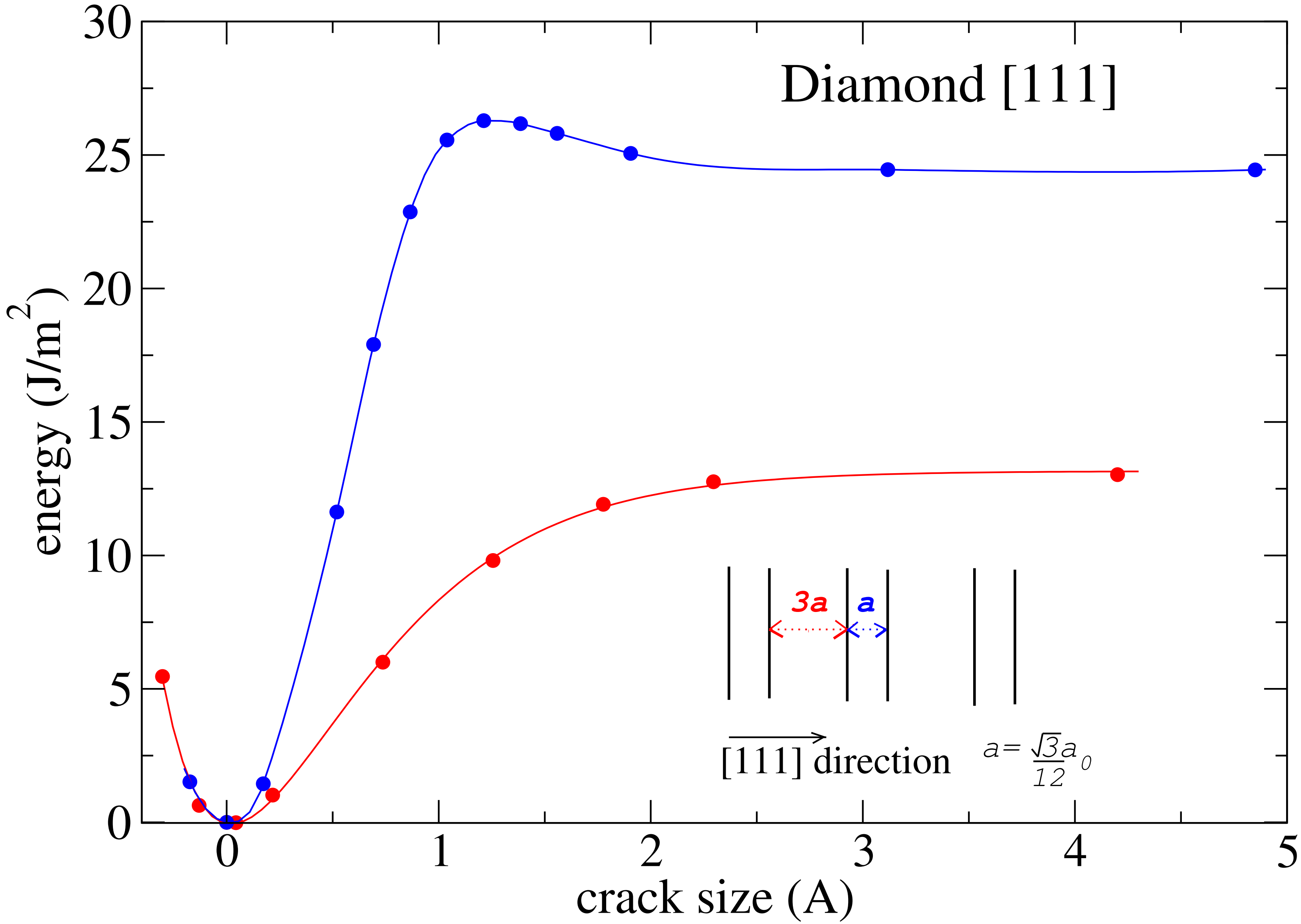
1. using idea of localisation of the elastic energy just at the point of rupture of material a simple formula

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

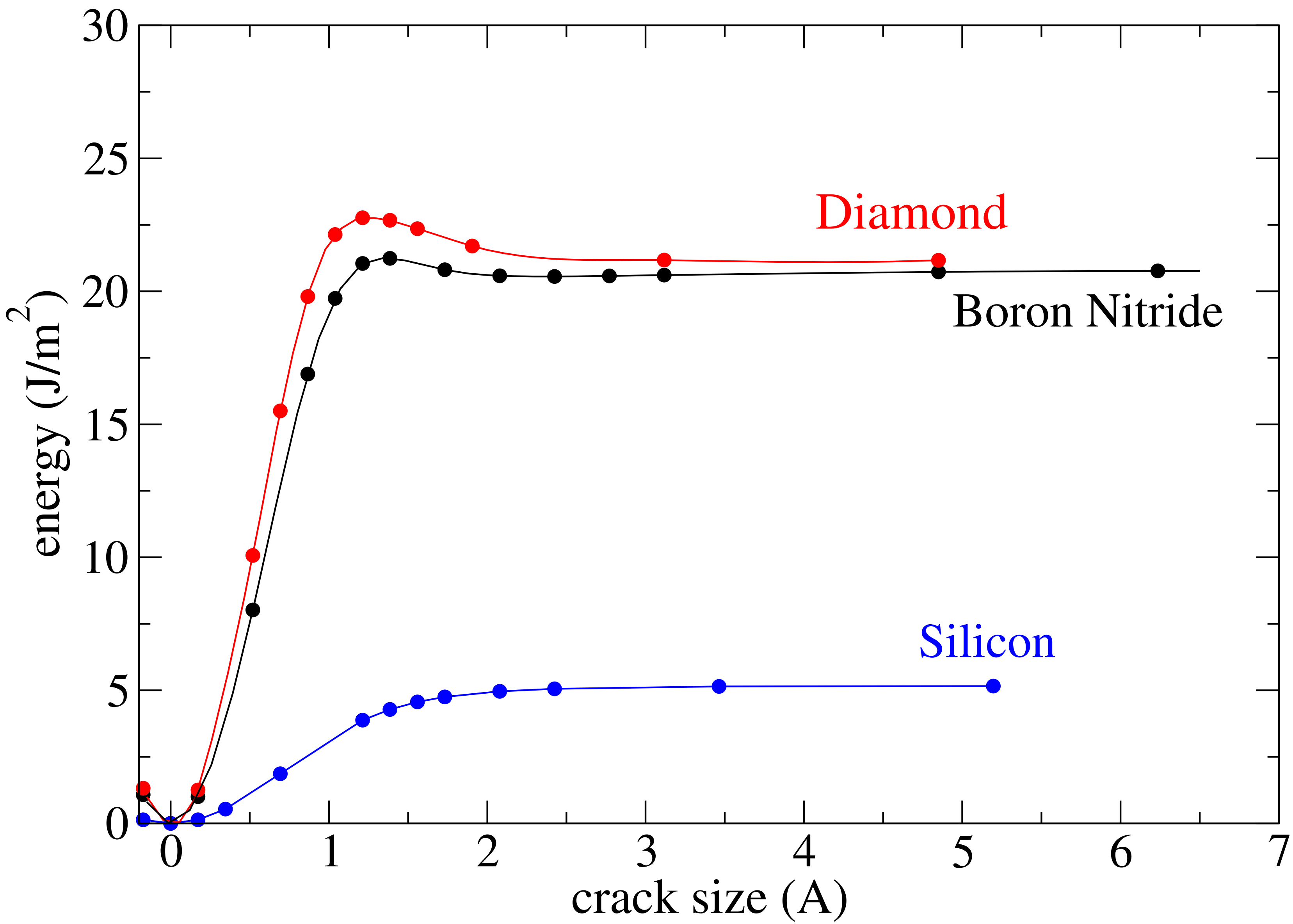
for estimate maximum cleavage stress just via cleavage energy, elastic constant was obtained. A new parameter L_b - localisation length - was introduced.

2. localisation length in the brittle limit L_b was found rather material and direction independent in all cases inspected. This allow to estimate maximum cleavage stress just using macroscopic material constants.

3. interesting correlation between critical separations in both limits was found



Diamond [111]
energy (J/m^2)
crack size (A)
0
5
10
15
20
25
30
0
1
2
3
4
5
3a
a
[111] direction
$a=\frac{\sqrt{3}a_0}{12}$



Diamond
Boron Nitride
Silicon
energy (J/m^2)
crack size (A)
0
5
10
15
20
25
30
0
1
2
3
4
5
6
7