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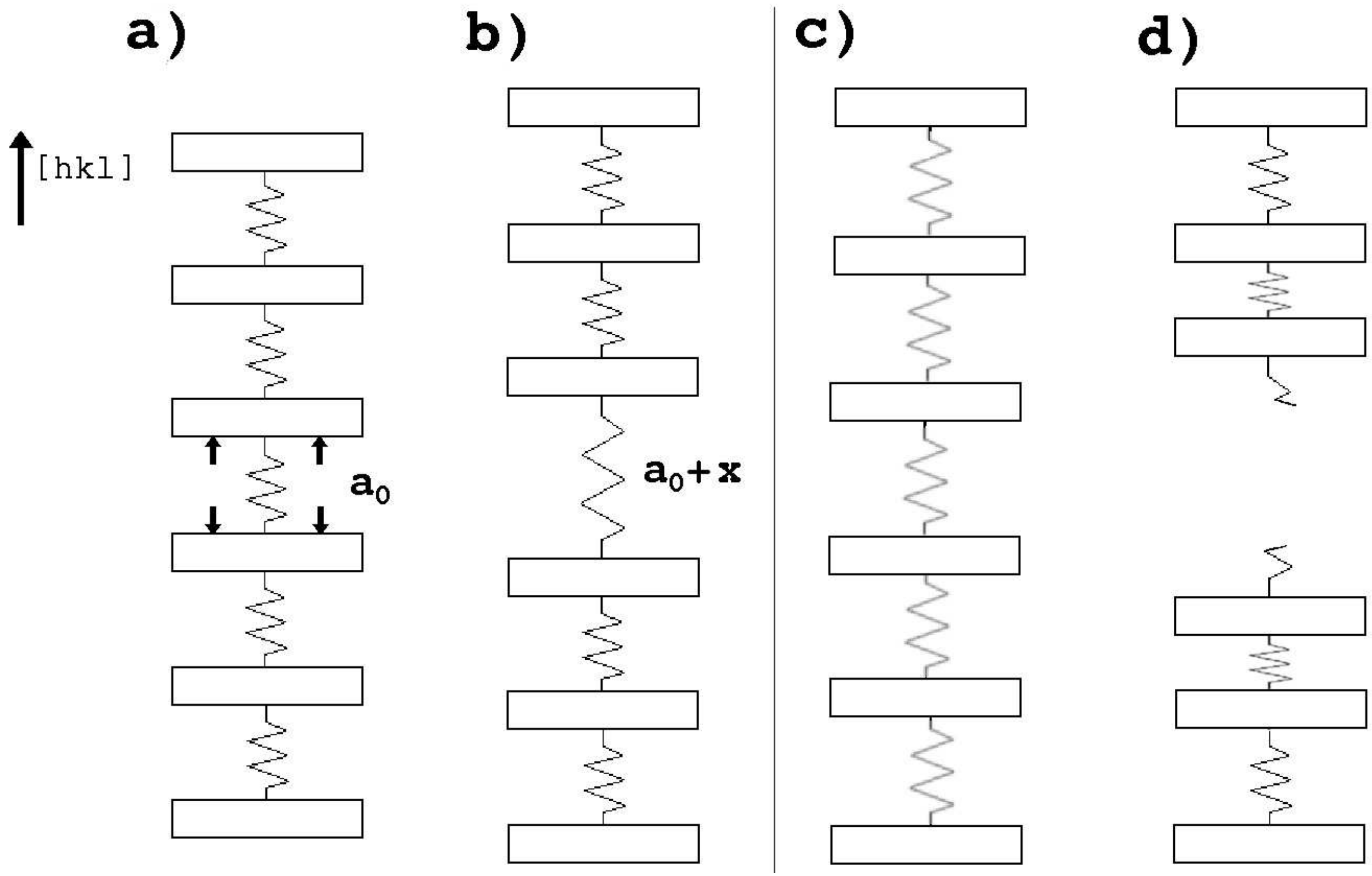
[1] M. Polanyi, Z. Phys **7**, (1921)
[2] E. Orowan, Rep. Prog. Phys. **12** (1949)
[3] J. J. Gilman, The strength of ceramic solids (Gordon & Breach, New York, 1963)
[4] M. H. Yoo and C. L. Fu, Mat. Sci. Eng, **A153** (1992)

Crack model:



b) Brittle case - in this simple model energy scales with separation 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)

c) Elastic case - energy follows separation as $E(x) = \frac{1}{2}Ac_{11}\frac{x^2}{L}$ until a relaxed value of cleavage energy G_e is reached - this is a critical point l_e where the crack is opened.

Therefore we can put

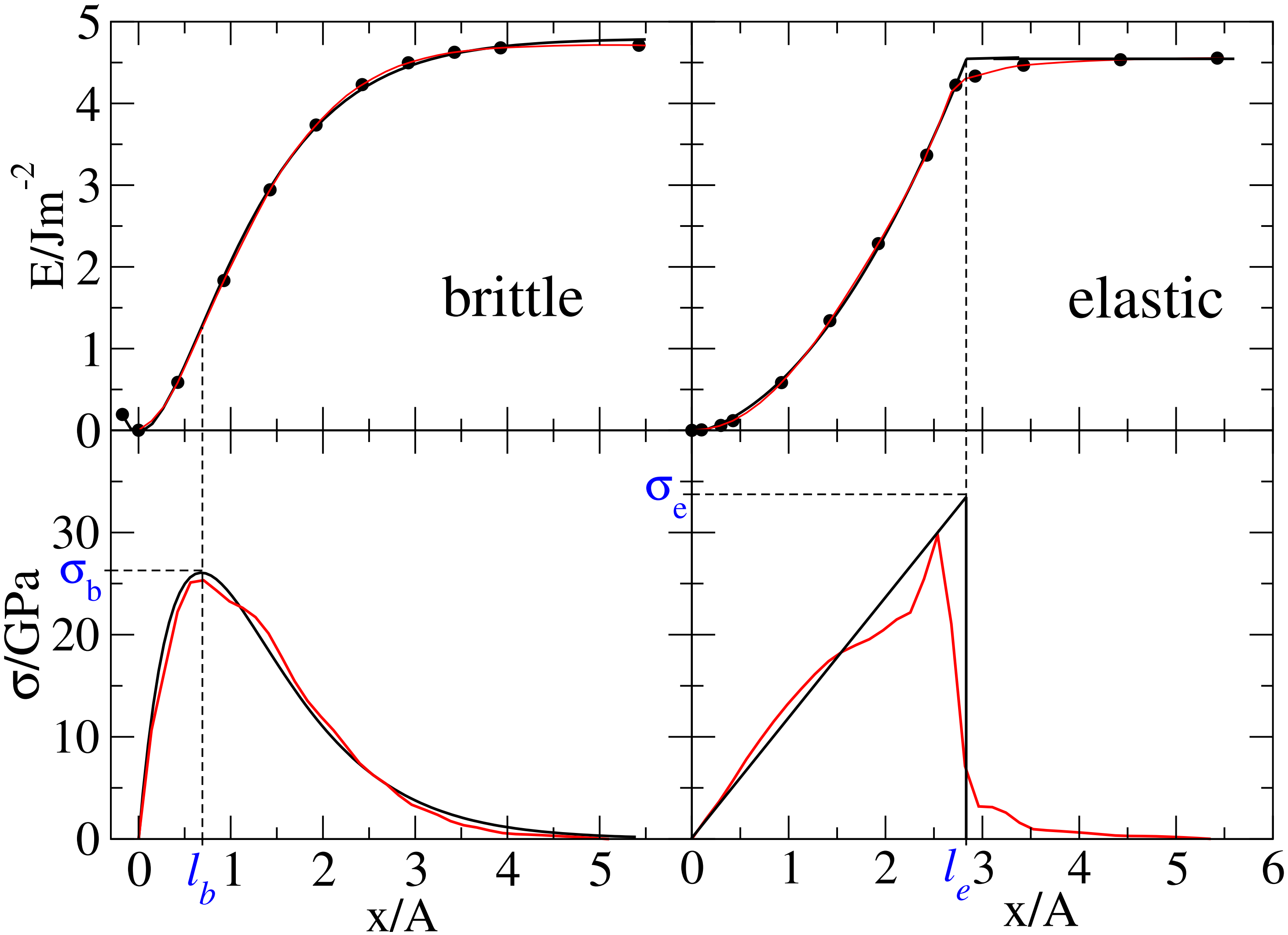
$$G_e = \frac{1}{2}Ac_{11}\frac{l_e}{L}$$

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
σb
σe
lb
le
x/A
x/A

Connecting elasticity and fracture - key assumptions:

I. at a critical limit $x = l_b$ (a point where the bonds are just about to break) elastic response and cleavage are at an unstable equilibrium, the elastic energy is localised in a local volume $V = AL_b$.

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

This quantity is rather constant, independent of material and direction!!!

II. at equilibrium, the energy of the brittle fracture has same curvature as elastic energy

$$\frac{1}{2}AG_b\frac{x^2}{l_b^2} = \frac{1}{2}AL_bc_{11}\frac{x^2}{L_b^2}$$

where left side of equation is Taylor expansion of UBER up to the second-order.

Then l_b in exact expression for critical stress $\sigma_b = \frac{G_b}{el_b}$ can be substituted!

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

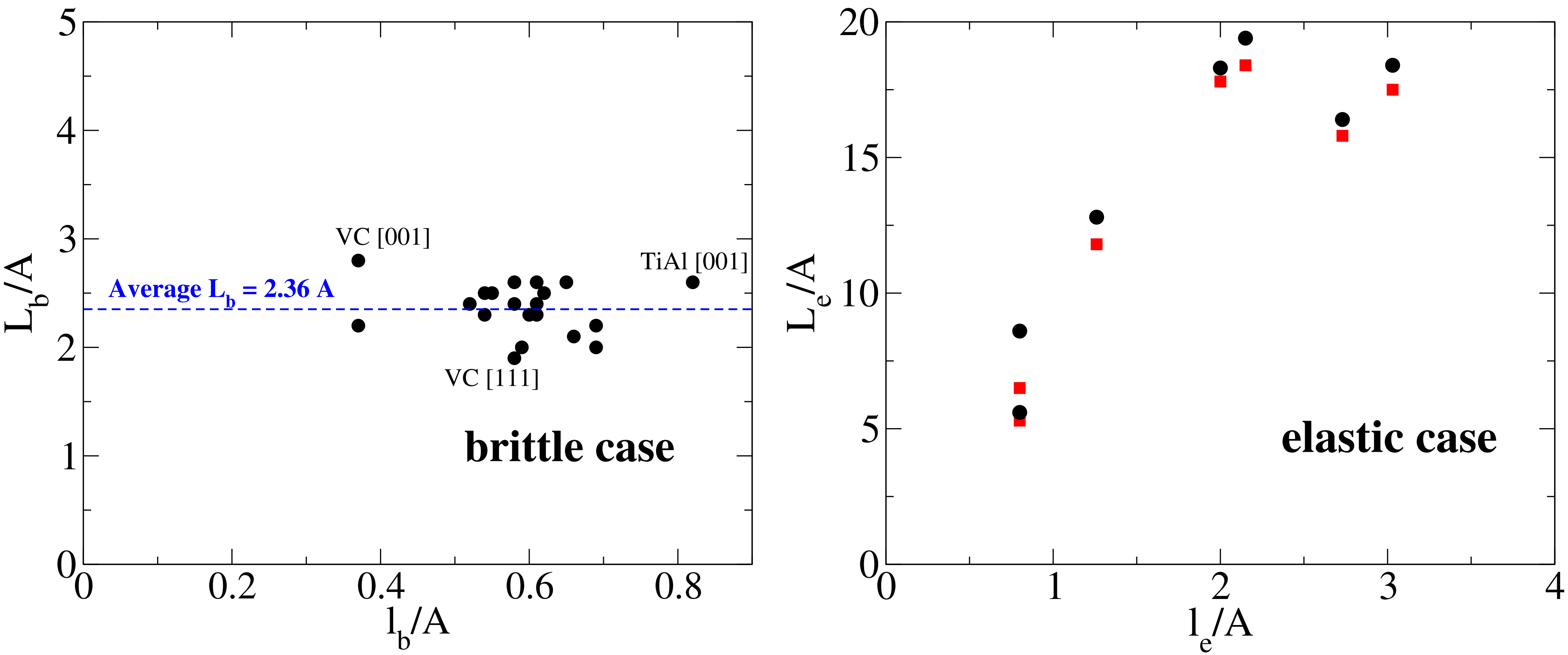
Calculated values - brittle limit

	direction $[hkl]$	c'_{11} GPa	G_b J/m^2	l 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
FeAl	001	278	5.7	0.69	31	2.2
	011	354	4.7	0.60	31	2.3
	111	380	6.1	0.62	36	2.5
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
Ni_3Al	001	225	4.3	0.66	24	2.1
	111	331	3.7	0.52	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
Iron	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

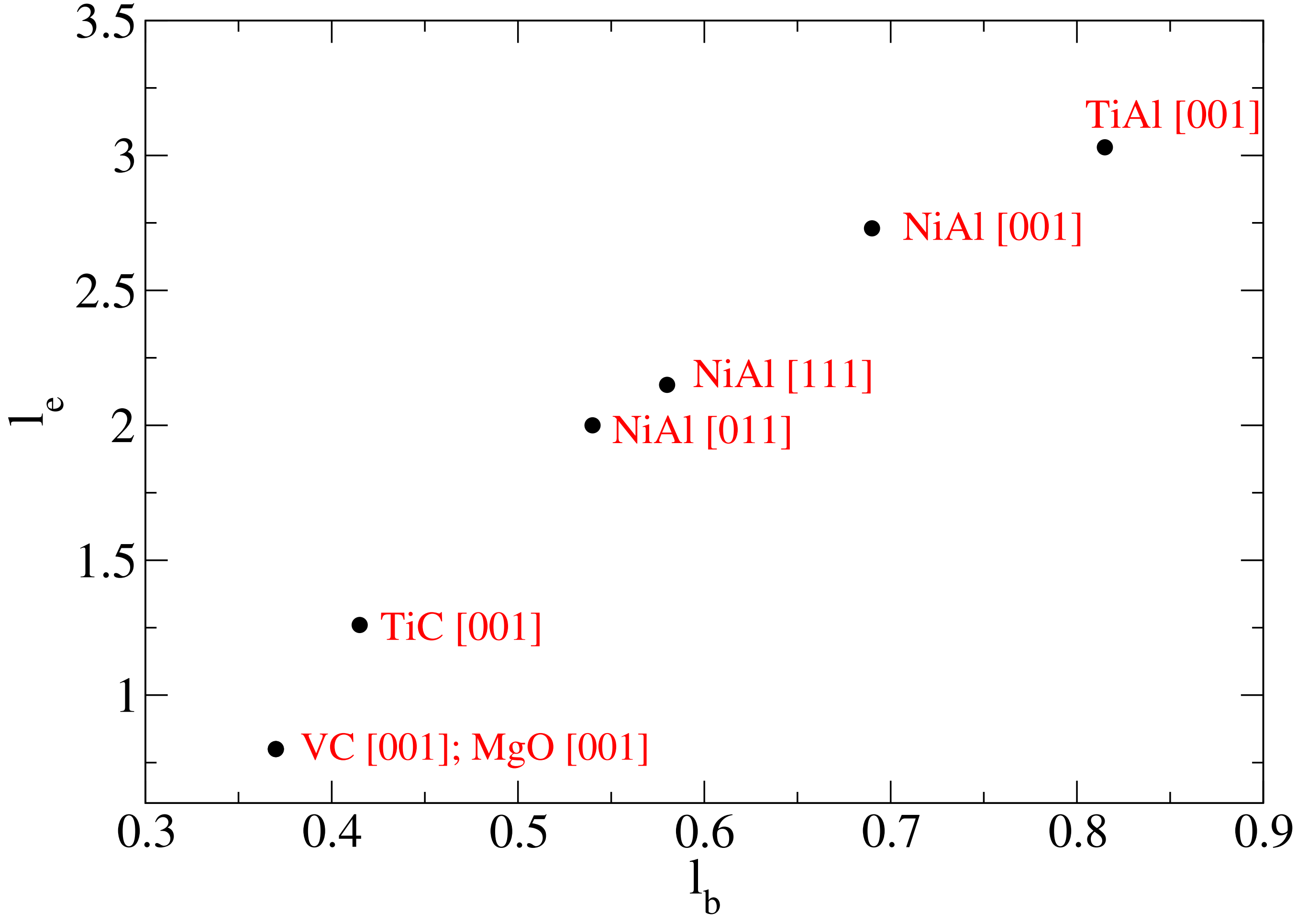
Elastic limit

	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

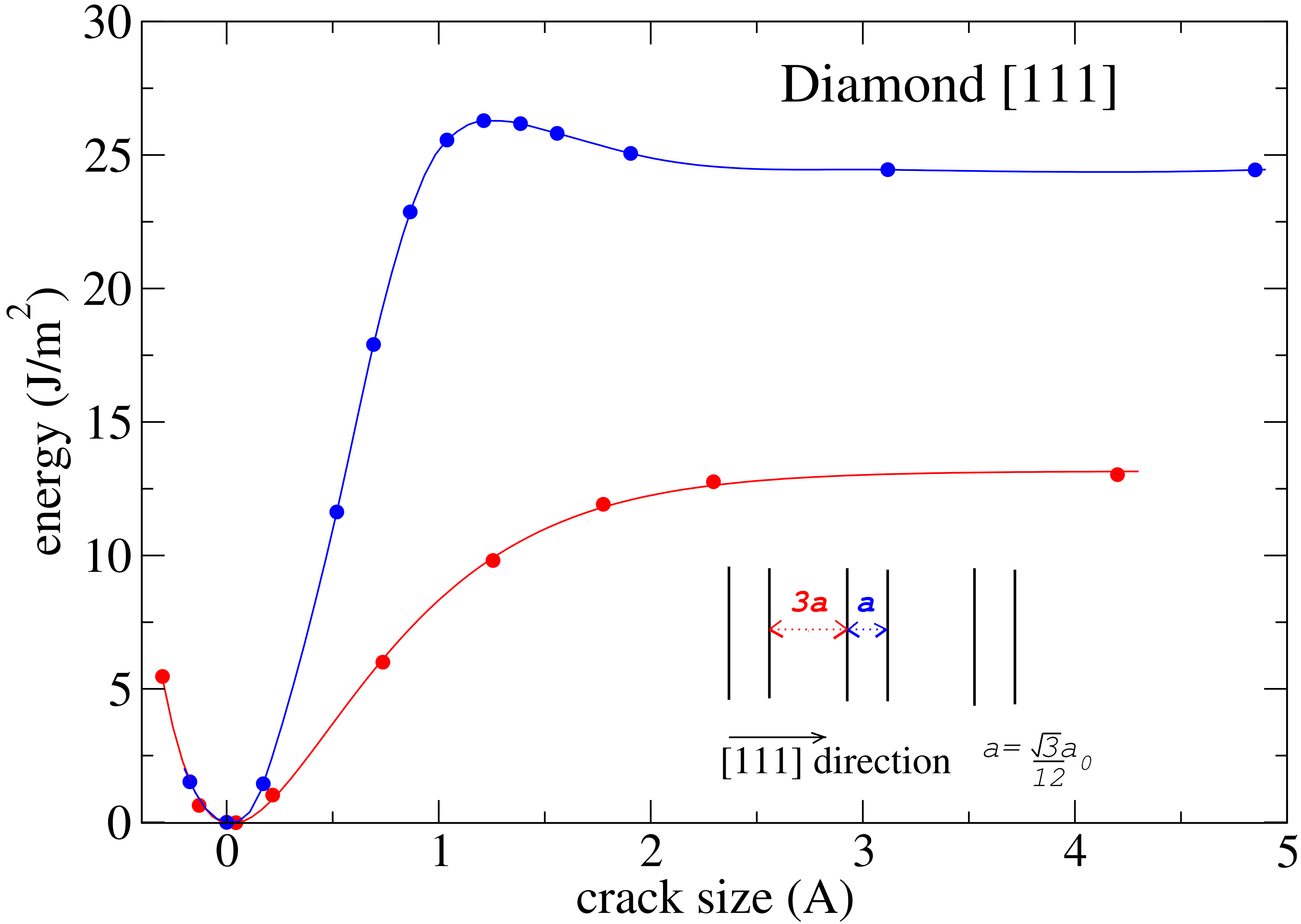
1. using idea of localisation of the elastic energy just at the point of rupture of material a simple formula

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

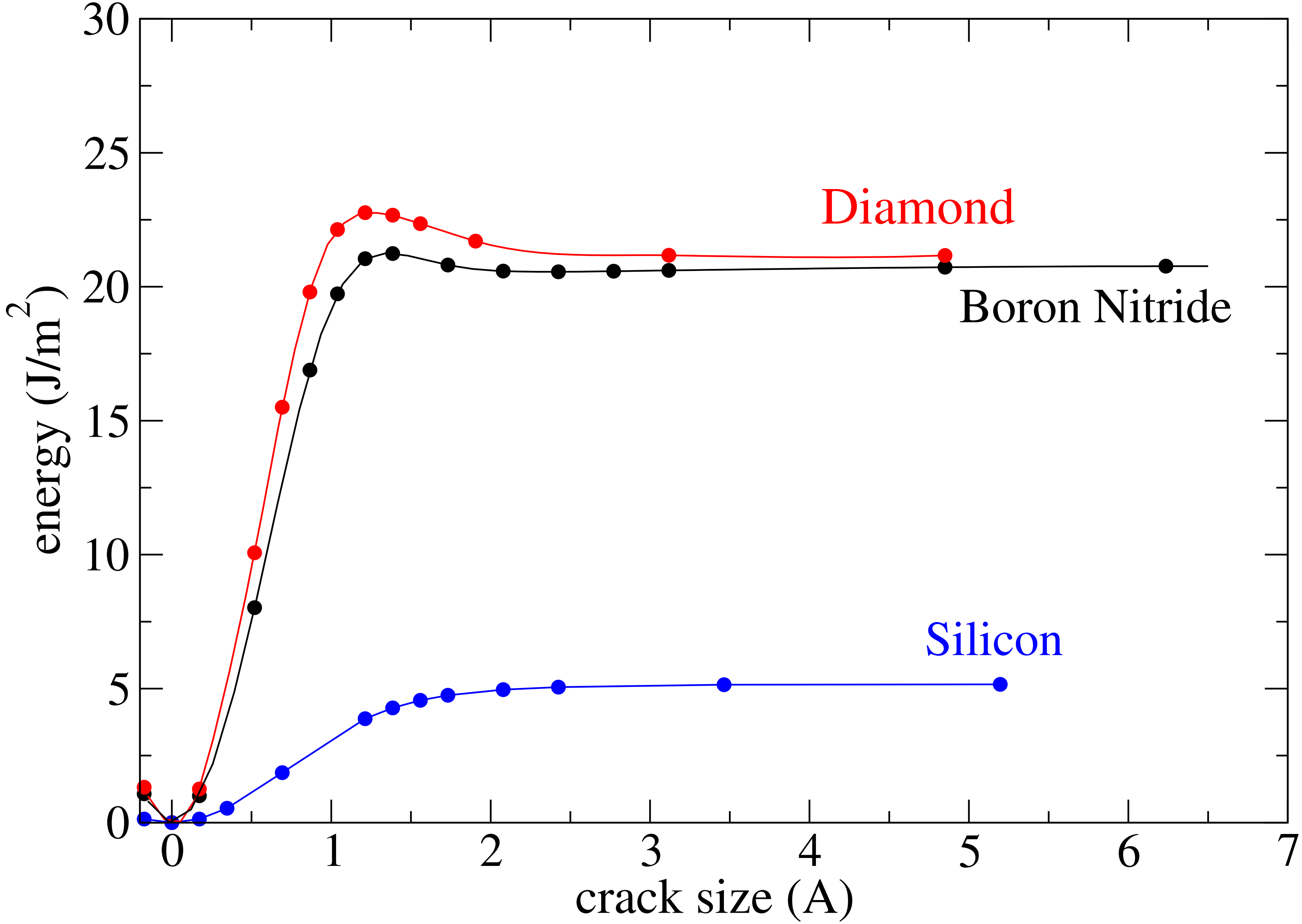
   for estimate maximum cleavage stress just via cleavage energy, elastic constant was obtained. A new parameter L_b - localisation length - was introduced.

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