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 formula overestimates theoretical cleavage stress

3. used even in ab-initio calculations[3]

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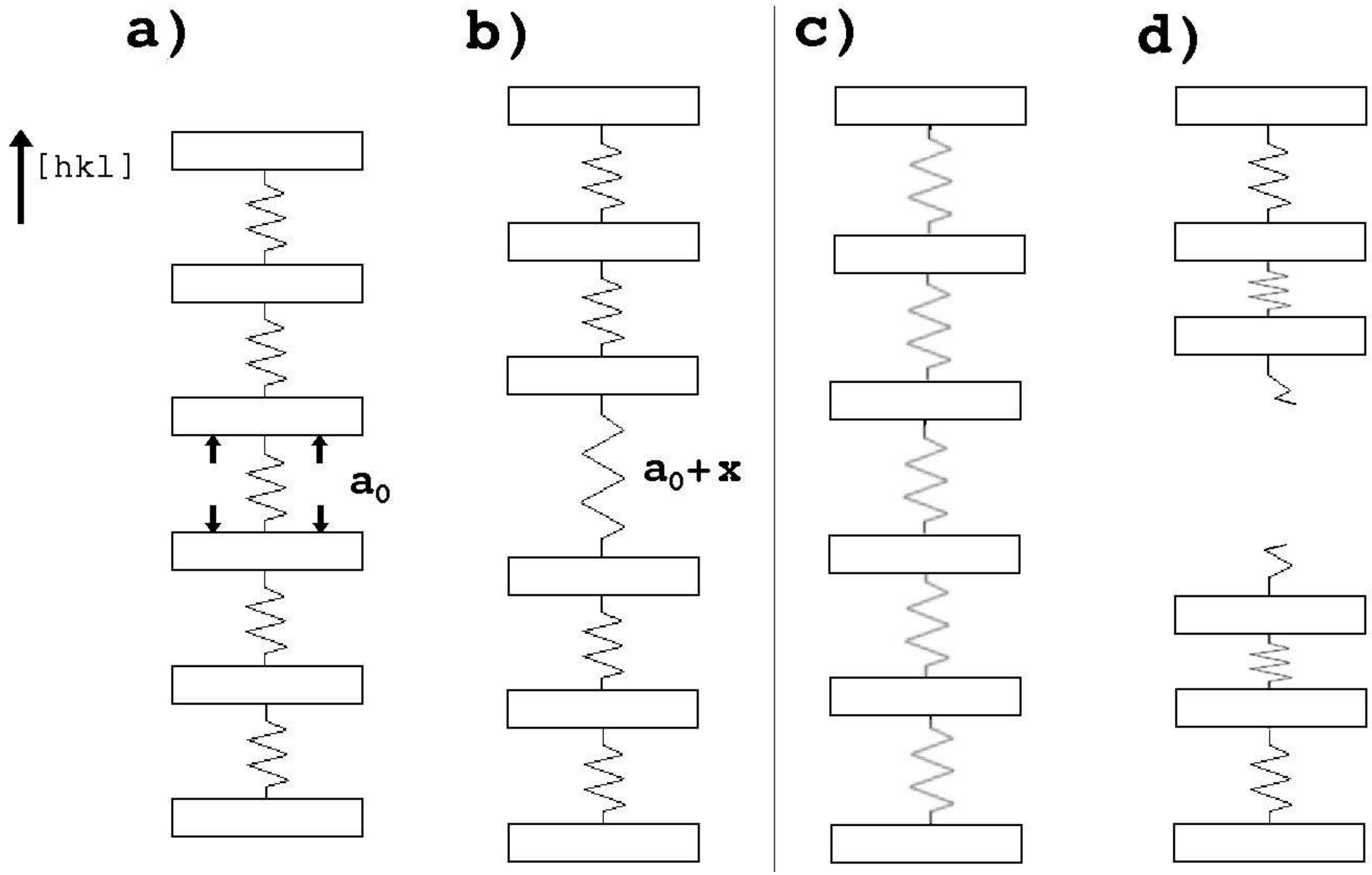
[1] M. Polanyi, Z. Phys **7**, (1921)
[2] E. Orowan, Rep. Prog. Phys. **12** (1949)
[3] M. H. Yoo and C. L. Fu, Mat. Sci. Eng, **A153** (1992)

Crack model:



For rigid block separation energy scales with x as (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

The 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, initial crack closed until a relaxed value of cleavage energy G_e is reached.

At the critical point l_e

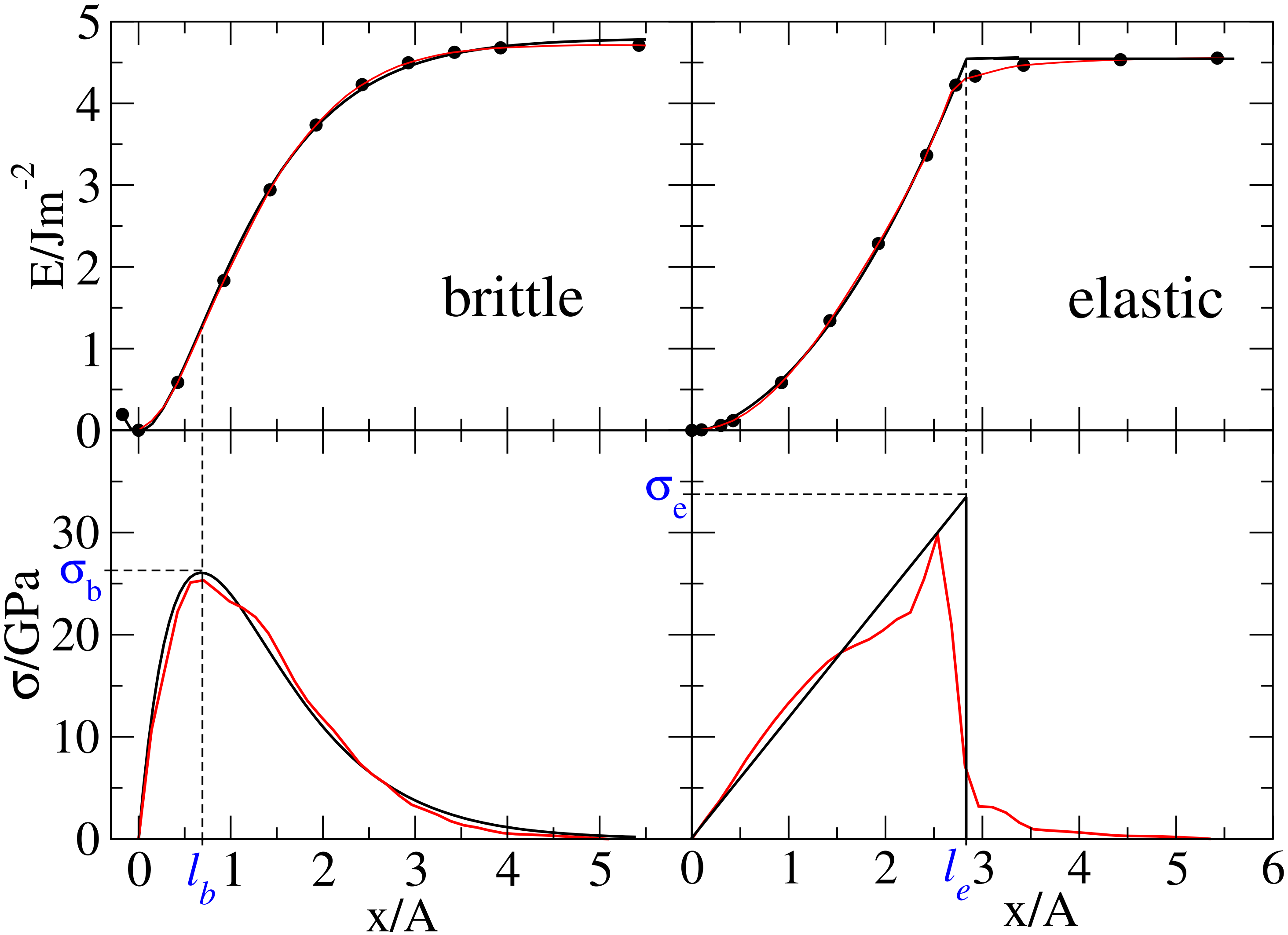
$$G_e = \frac{1}{2} A c_{11} \frac{l_e}{L}$$

Elastic energy

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

Maximum of the stress in the elastic limit

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



E/Jm^{-2}
brittle
elastic
σ/GPa
σ_b
σ_e
l_b
l_e
x/A
x/A
0
1
2
3
4
5
0
10
20
30
0
1
2
3
4
5
6

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} [5]

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

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

	$[hkl]$	l_b Å	L_b Å	l_e Å	L_e Å
NiAl	001	0.69	2.0	2.7	15.8
	011	0.54	2.5	2.0	17.7
	111	0.58	2.4	2.2	18.4
TiAl	001	0.82	2.6	3.0	17.5
VC	001	0.37	2.8	0.8	6.5
MgO	001	0.37	2.2	0.8	5.3
TiC	001	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

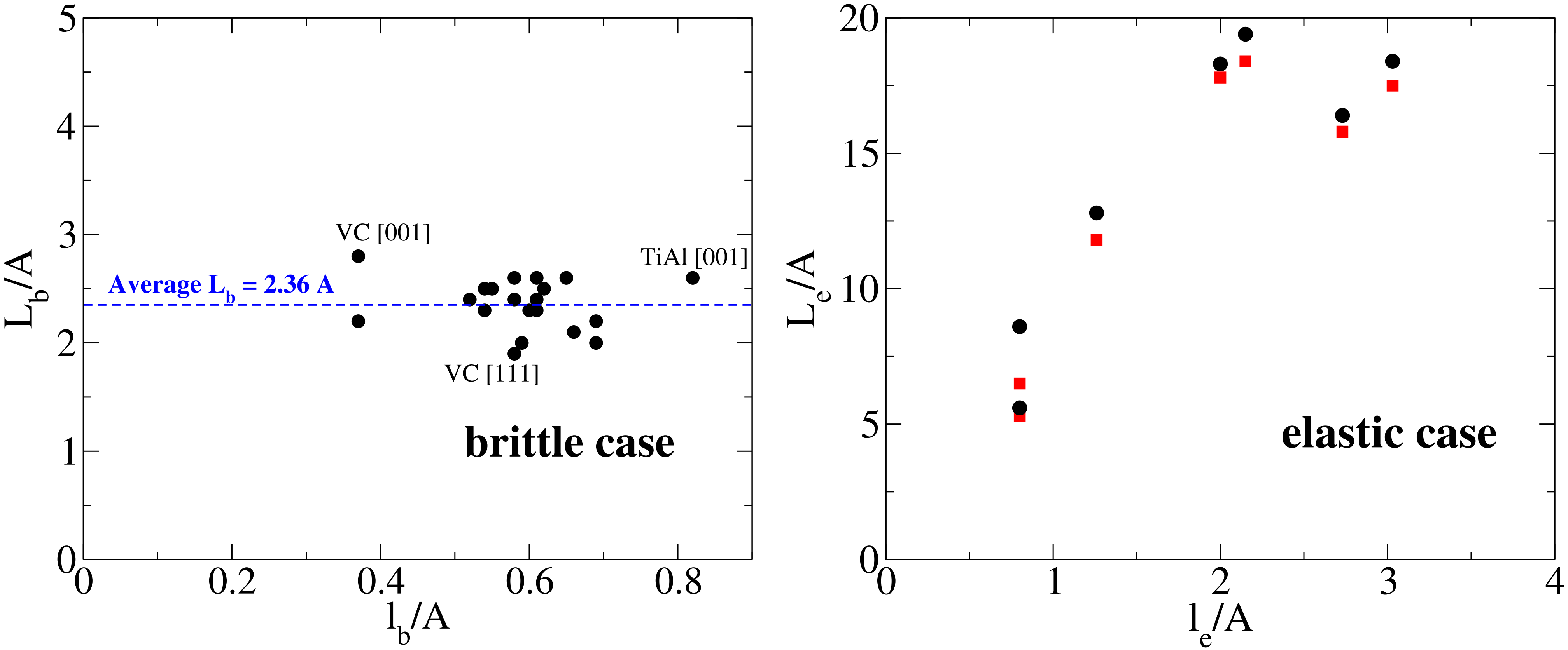
Calculated values - brittle limit

	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**

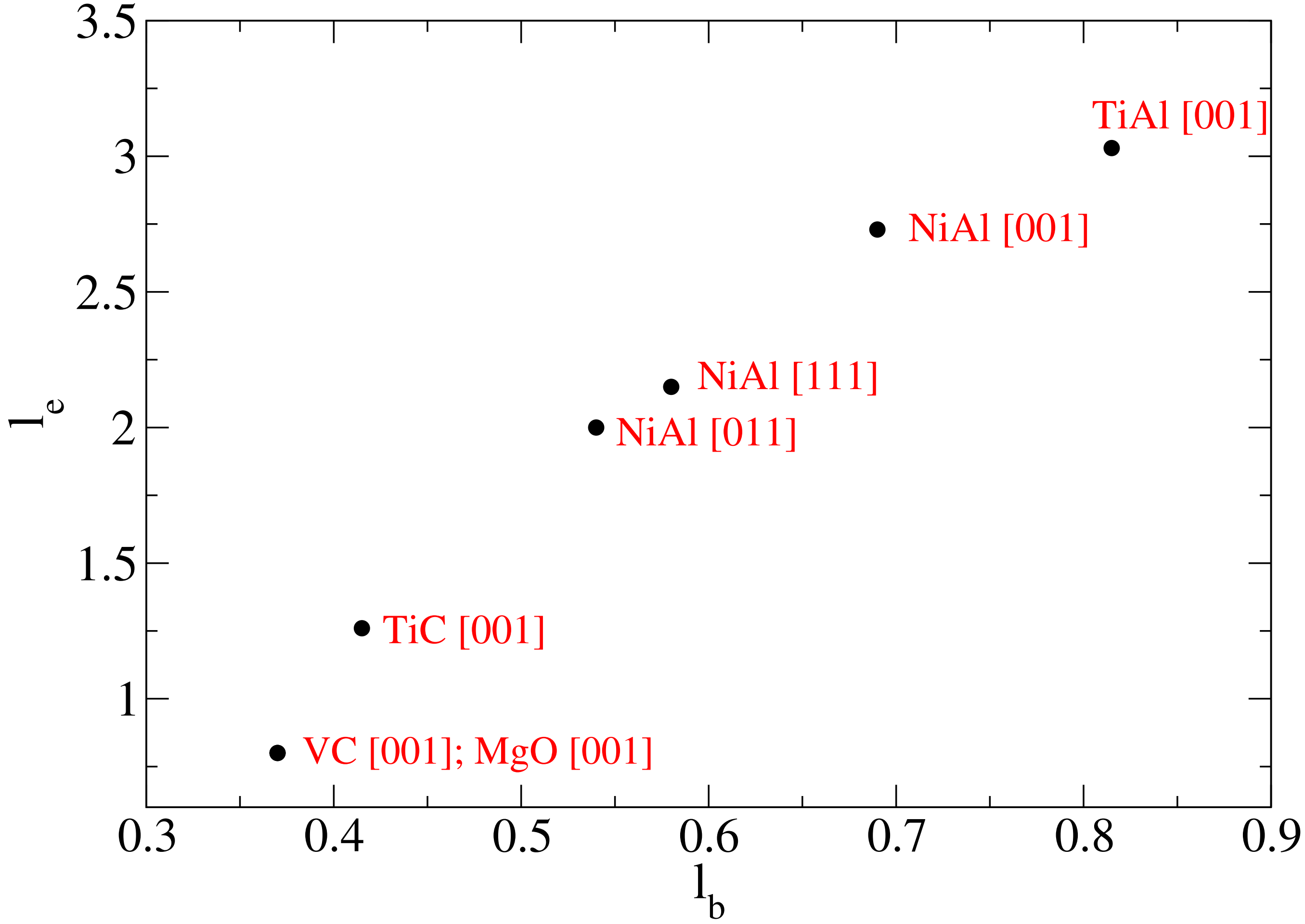
Elastic limit

	direction $[hkl]$	G_e (J/m^2)	l_e ($\AA$)	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. simple analytic formula for crack in the elastic limit was derived

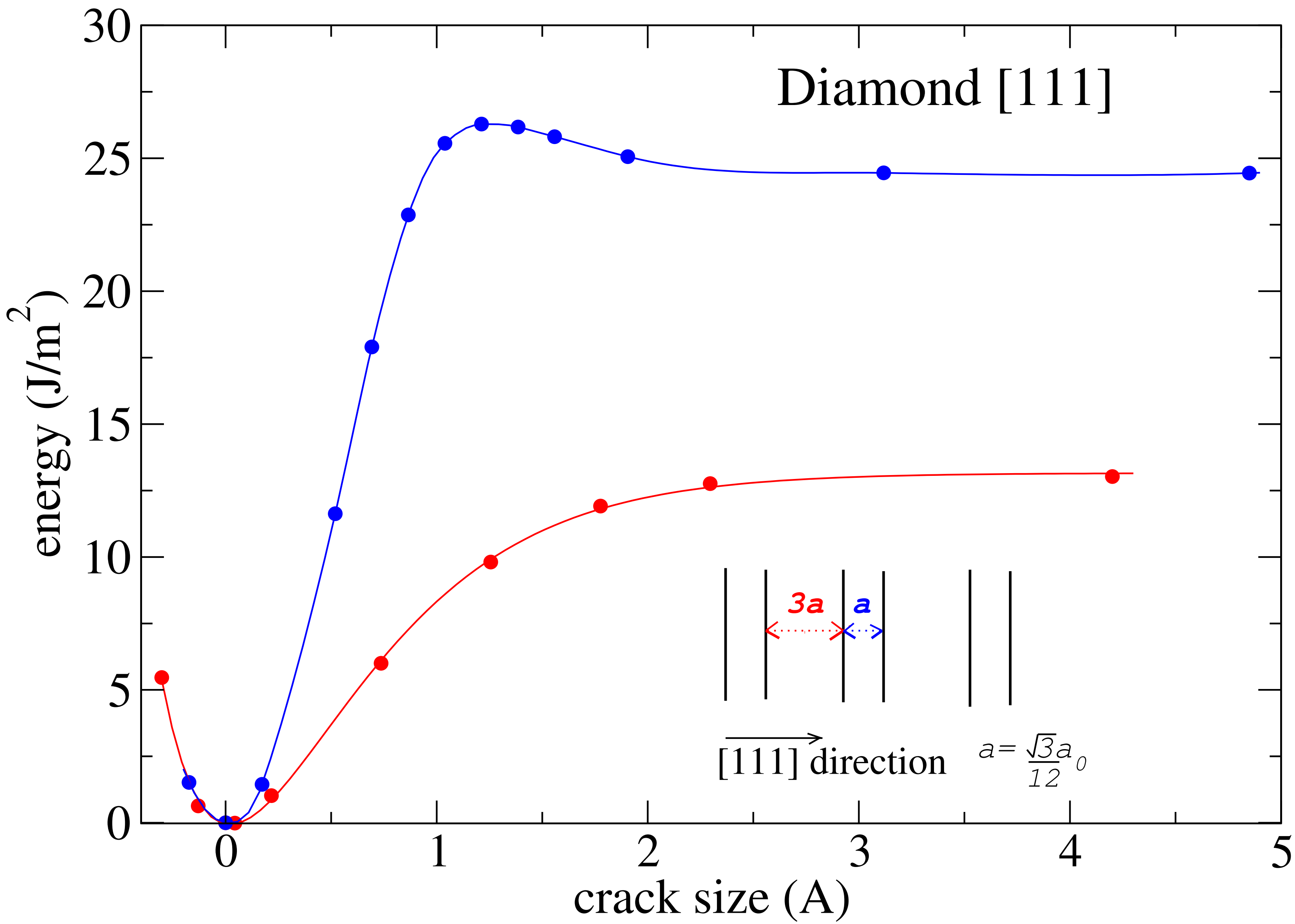
$$E(x) = G_c \frac{x^2}{l_e^2}$$

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

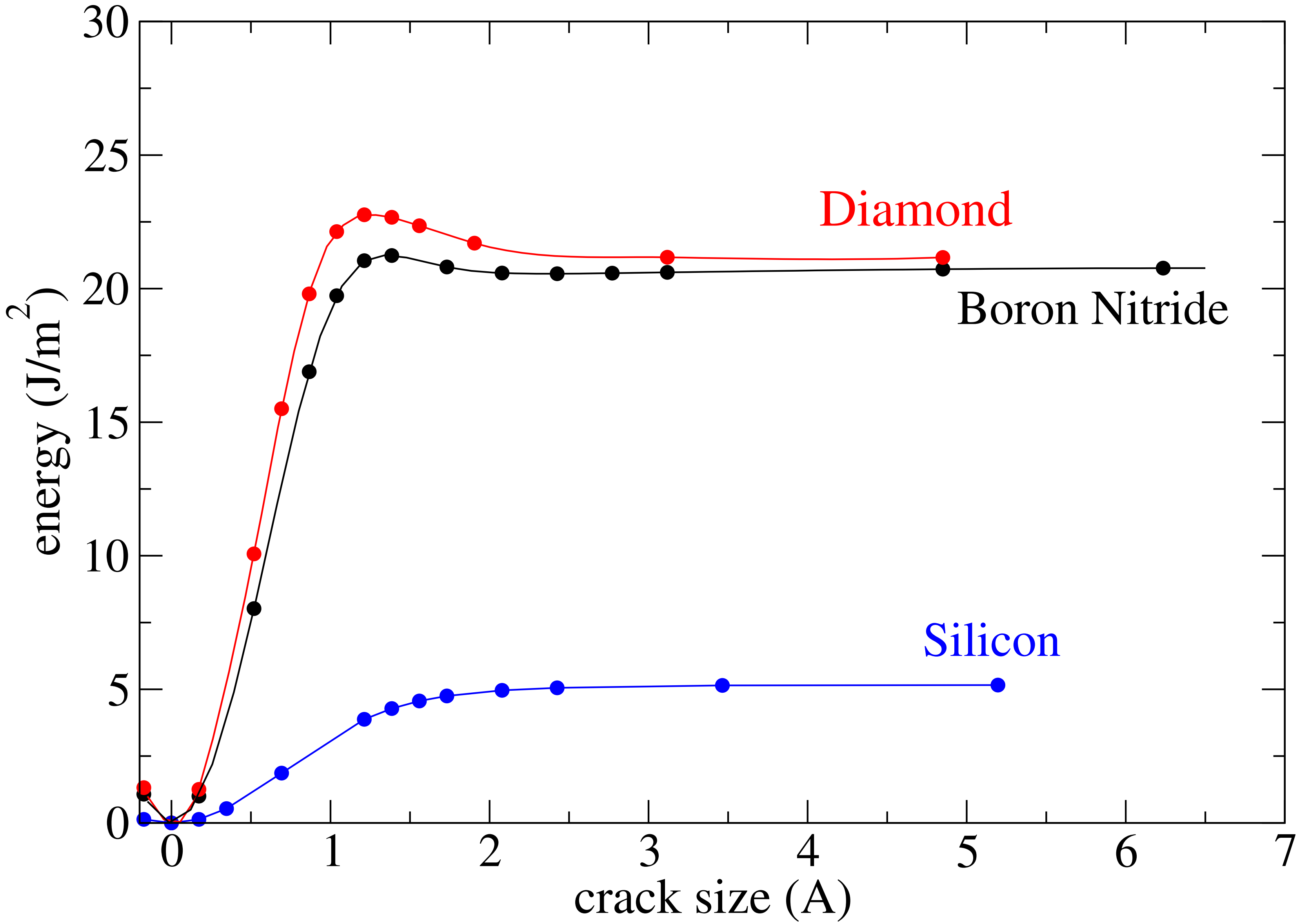
$$\sigma_b = \frac{1}{e}\sqrt{\frac{G_b c_{11}}{L_b}}$$

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

3. localisation length in the brittle limit L_b was found rather material and direction independent in all cases inspected.



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
$a = \frac{\sqrt{3}a_0}{12}$



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