Computational Materials Physics

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what are elastic constants used for ?

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http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

Several so-called "elastic moduli" can be derived from the elastic constant.

For cubic crystals:

Bulk modulus B: $B = \frac{c_{11} + 2\,c_{12}}{3}$

Shear modulus G: $G = \frac{c_{11} - c_{12} + 3\,c_{44}}{5}$

Young's modulus E: $E = \frac{9BG}{3B + G}$

micro-hardness Hv: $H_V = (1 - 2\nu)\,E / [6\,(1 + \nu)]$
with $\nu = (3B - 2G) / [2\,(3B + G)]$

Speed of sound

Longitudinal: $v = \sqrt{\frac{B + \frac{4}{3}G}{\rho}}$

Shear: $v = \sqrt{\frac{G}{\rho}}$

Typical agreement with experiment (here for fcc Cu) :

	Our calculations	Experiment
Lattice constant [Å]	3.64	3.61 [1]
C_{11} [GPa]	176.7	176.20 [2]
C_{12} [GPa]	122.4	124.94 [2]
C_{44} [GPa]	78.0	81.77 [2]
Speed of sound [m/s]	4403	4439.5 [2]
Melting temperature [K]	1577	1356 [3]
Bulk modulus [GPa]	137.1	142.0 [2]
Shear modulus [GPa]	57.66	59.3 [2]
Young's modulus [GPa]	151.7	156.2 [2]
Poisson's Ratio	31.9%	31.7% [2]

(Taken from an exam by Yves Beghein, Jan Jaeken and Steven Vandenbrande)

Born stability criteria:
Eigenvalues of the C-tensor must be positive

Example for the cubic case:

$$c_{11} > 0$$
$$c_{44} > 0$$
$$c_{11}-c_{12} > 0$$
$$c_{11}+2c_{12} > 0$$

Even if E_{coh} is positive (energetically stable),
the material might not be mechanically stable

Up to now, we discussed elastic constants at p=0. Just as the bulk modulus, they can be generalized to any pressure.