Center for Molecular Modeling

Computational Materials Physics

Department of Materials Science and Engineering

bulk modulus and pressure

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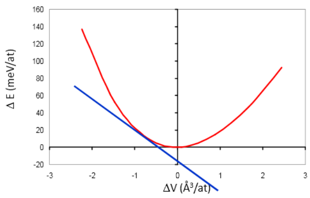
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

Bulk modulus B = pressure change required to realize a given relative volume change, at a given volume.

$$B_0 = -\frac{\Delta p}{\frac{\Delta V}{V_0}} = -\frac{p-0}{\frac{V-V0}{V_0}} = -V_0\frac{\Delta p}{\Delta V} = -V_0\frac{\partial p}{\partial V} = V_0\frac{\partial^2 U}{\partial V^2}$$

$$dU(S,V) = TdS - pdV$$

$$\frac{\partial U}{\partial V}(S,V) = -p$$



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at equilibrium

$$= -\frac{p-0}{\frac{V-V0}{V_0}} = -V_0\frac{\Delta p}{\Delta V} = -V_0\frac{\partial p}{\partial V} = V_0\frac{\partial^2 U}{\partial V^2}$$

B can be defined at any other volume (or pressure) too
➔ B is pressure dependent

$$B(p) = B(0) + B'p + \frac{1}{2}B''p^2 + \ldots$$

$$= B_0 + B_1 p + \frac{1}{2}B_2 p^2 + \ldots$$

at equilibrium

Other equations of state:

Birch-Murnaghan (valid up to 10% volume change):

http://en.wikipedia.org/wiki/Birch%E2%80%93Murnaghan_equation_of_state

$$P(V) = \frac{3B_0}{2}\left[\left(\frac{V_0}{V}\right)^{\frac{7}{3}} - \left(\frac{V_0}{V}\right)^{\frac{5}{3}}\right]\left\{1 + \frac{3}{4}\left(B_1 - 4\right)\left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]\right\}$$

$$E(V) = E_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^3 B_1 + \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^2\left[6 - 4\left(\frac{V_0}{V}\right)^{\frac{2}{3}}\right]\right\}$$

From Physical Review B 52 (1995) 8064 ("eos2"):

$$E = a + bV^{-1/3} + cV^{-2/3} + dV^{-1}$$

Useful paper: Ronggang 2010 (http://stacks.iop.org/PhysScr/82/045014)

Comprehensive yet accessible book: Anderson 1994 (http://books.google.be/books/about/Equations_of_State_for_Solids_in_Geophys.html?id=qSqiz2NK7TIC)

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accuracy of V_0, B_0 and B_1

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