

Abstract Submitted
for the SHOCK05 Meeting of
The American Physical Society

The Bond Modulus and the Stability of Solids JOHN GILMAN,
UCLA — The chemical stabilities of molecules are determined by their LUMO-HOMO energy gaps. For solids the of these are their energy band gaps. However, solids are poly-molecules (i.e., polymers). But, the stabilization energy of a monomer cannot be used to describe the stability of a polymer. An intensive para-is needed. Such a parameter is the gap energy per molecular volume. The author has coined the name “bond modulus” for this parameter because it tends to be proportional to elastic moduli and it has the same dimensions. It applies primarily to covalent solids with localized bonding (i.e., Group IV elements, III-V, and II-VI compounds. A related parameter is electronegativity difference density. It correlates mobilities, indentation hardnesses, and critical compressions for structure transformations. It is proportional to chemical hardnesses, and bulk moduli, as well as octahedral shear moduli, and inverse polarizabilities.

John Gilman
UCLA

Date submitted: 09 Mar 2005

Electronic form version 1.4