Useful microscopic concepts for high pressure phenomena[1]

J. MANUEL RECIO, J. MANUEL MENÉNDEZ, RUTH ÁLVAREZ-URÍA, MIRIAM MARQUÉS, Malta-Consolider Team and Universidad de Oviedo, TARIK OUAHRANI, University Abubakr Belkaid, VALENTÍN G. BAONZA, Malta-Consolider Team and Universidad Complutense de Madrid — A better understanding of the macroscopic behavior of crystalline solids under pressure can be achieved introducing microscopic concepts as the local compressibility ($\kappa_i=-\frac{1}{V}\frac{\partial V}{\partial p}$) and the local pressure ($p_i=-\frac{\partial E}{\partial V_i}$). Both are derived from topological analysis of crystalline electron densities. This formalism allows for a partition of the unit cell volume (V) into disjoint atomic-like regions such that $V=\sum_i V_i$, i runs over all different atomic constituents. Using this topological partition, the compressibility of the crystal is recovered: $\kappa=\sum_i \frac{V_i}{V}\kappa_i$. Although local pressures are not additive, their reciprocals are: $\frac{1}{p}=\sum_i \frac{1}{p_i}$, where p is the thermodynamic pressure. This fact leads to the interpretation of the atomic constituents of crystals as parallel mechanical resistors when pressure is applied. Consequently, atomic-like mechanical resistances and mechanical conductances can be defined. After extensive first principles calculations, computed results of these local properties reveal systematic trends for crystal families under pressure, as we illustrate for II-VI binary semiconductors and oxide spinels.

J. Manuel Recio
Malta-Consolider Team and Universidad de Oviedo

Date submitted: 25 Feb 2013　　　　　　　　　　　Electronic form version 1.4