

Homework 3: Computational Design of Materials

Due: Nov. 30, 2012

1. As discussed in our class, the Cauchy pressure defined as $C_{12}-C_{44}$ is typically positive for non-directional metallic bonding (ductile) compounds (the Pettifor's criterion). The larger positive value represents a more metallic bonding. The negative value signifies a covalent bonding framework. On the other hand, materials with $G/B > 0.57$ behaves in a brittle manner (the Pugh's criterion), the higher the value of G/B , the more brittle the materials.

Based on these guidelines, let us investigate the following materials: Pb (FM-3M), Si (FD-3M), c-BN (F-43M) and Diamond (FD-3M) by calculating their elastic properties with first-principles method. Present your results on the plot of $(C_{12}-C_{44})/E$ as a function of G/B . Discuss their structural and bonding nature and explain the origin of hardness in these materials.