What we can learn from the mechanical behavior of glasses about their atomic and molecular structures

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The mechanical properties of glasses from different chemical systems were studied in the light of the atomic packing density (C_g), medium range order and atomic bonding character. The elastic moduli reflect the volume density of energy, and are thus directly correlated to C_g and to the bond strength. Nevertheless, the packing density has actually the greater influence on the final result. The same conclusion is drawn for hardness. As a matter of fact, the hardest and stiffest glasses are not those with the strongest interatomic bonding! In the case of metallic glasses, we found that the electronegativity mismatch (Δe-) between the host- and the major solute - elements provides a plausible explanation to the large variation observed for Poisson's ratio (ν) notwithstanding a similar C_g. This correlation also holds for monoconstituent oxide glasses and hence provides an explanation to the variation of ν observed for seemingly "isostructural" glasses. In the search for more ductile glasses, the bond directionality and the sensitivity to volume change are key parameters. The energy required for a stable crack propagation through the system, where the crack tends to follow the easy paths, provides some insight into the energy landscape, with a remarkable consistency between the energy as calculated from the bond density and from self-consistent fracture toughness measurements. The presence of weak channels favoring shear flow can also be invoked to interpret the temperature sensitivity of the viscous flow (fragile versus strong liquids). Finally, the problem of crack initiation from a sharp contact loading is also discussed with respect of the possible deformation mechanisms, which are further correlated with the atomic organization.

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