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Bond enthalpy trends of high metalloid Fe-based bulk metallic glasses M. WIDOM, B. SAUERWINE, Carnegie Mellon University, N. KVALTINE, X.J. GU, S.J. POON, G.J. SHIFLET, University of Virginia — Chemical bond types in metal-metalloid glass-forming compounds range from metallic to ionic and covalent. Iron-rich alloys are dominated by metallic bonding, but charge transfer from iron atoms to highly electronegative metalloid elements such as boron, carbon and phosphorous creates ionicity, and the metalloid bonding is intrinsically covalent. For sufficiently large metalloid content their strong bonding character must increase the shear modulus, leading to an associated increase in brittleness of the material. However, for metalloid fractions below 30%, shear modulus is found to decrease with increasing metalloid content, leading to an associated increase in ductility of the material. We show this unexpected decrease in shear modulus is caused by depletion of the charge density around the iron atoms, weaking the iron-iron bonds. Our calculations are based on Crystal Orbital Hamilton Populations (COHPs) for crystalline structures that locally approximate the amorphous structure.

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