Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

**Theoretical study of the structural, mechanical, and electronic properties in hydrides** RYOJI SAHARA, BUN TSUCHIYA, HIROSHI MIZUSEKI, SHINJI NAGATA, TATSUO SHIKAMA, YOSHIYUKI KAWAZOE, Institute for Materials Research, Tohoku University — Although an understanding of the mechanical behavior such as elastic properties and hardness of hydrides is important for their applications, theoretical studies have received little attention and only recently some progress has been made. In the present study, first-principles calculations have been performed on hydrides of Ti, Zr, and Hf. The elastic properties are estimated as a function of hydrogen concentration. Equilibrium lattice constants and the bulk moduli are estimated using Murnaghan EOS. While, the elastic constants, shear moduli, and Young's moduli are estimated introducing the strain tensor. The origin of these properties is explained in terms of the changes in the bonding characters as well as cohesive energy. A semi-empirical relationship between the bulk modulus/shear modulus and the Vickers hardness is introduced to predict hardness of these materials from the present first-principles calculation results.

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Date submitted: 02 Dec 2007 Electronic form version 1.4