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Elastic Constants of Rare Earth and Transition Metal Di-Hydrides¹ C. S. SNOW, J. A. KNAPP, J. F. BROWNING, Sandia National Laboratories — Determinations of the elastic constants of rare earth (RE=Er, La,) and some transition metal (TM=Sc, Ti, Zr) di-hydrides are extremely difficult. Single crystals of these di-hydrided metals can not be obtained because they break up into fine powders due to the large stresses in the materials caused by the crystallographic changes upon hydriding. However, polycrystalline thin films of these hydrided materials can be grown and are stable over a wide temperature and pressure range. In order to determine the elastic constants of thin metal di-hydride films ab-initio electronic structure calculations using the VASP code have been carried out. These calculations are then compared to bulk and shear moduli measured by a nanoindentation technique. Details and results of the calculations and measurements of the elastic constants of rare earth and transition metal di-hydride films will be presented and a discussion of future applications of this technique will be given.

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