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Electrical Resistivity Studies of Order-Disorder Phenomena in V2H and V2D

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perhaps by the onset of hydride precipitation from the saturated solid solution, are believed to be due to the presence of energetically favorable interstitial sites, or "traps", in the vicinity of the substitutional Ti solute atoms. The magnitude of the TSH enhancements suggests that Ti is a more effective trapping center than Ta, but less effective than V. Proposed explanations for this behavior based upon electronic and atom-size considerations will be discussed.

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KJ 9 Phase Equilibrium and Hydrogen Trapping in Dilute Alloys of Vanadium in Niobium.* M. A. Pick and D. O. Welch, Brookhaven Nat'l Lab. -- The effect of dilute vanadium additions to niobium on hydrogen absorption was studied by measuring the temperature dependent equilibrium hydrogen partial pressure for pure Nb, Nb-5at.% V, Nb-9at.% V, and Nb-9at.% W. A theoretical model of the effect of hydrogen trapping on phase equilibria in the α-β region of such systems was constructed. The results indicate that the H-V binding energy is less than previously thought. A value of 0.07 eV is obtained from the depression of the α-β critical temperature, but the shape of the pressure isotherms suggests that this is an upper limit. The measured heat of solution decreases from -31.6 to -38.6 kJ-mol, going from pure Nb to Nb-6at.% V to Nb-9at.% W.

*Research supported by the Div. of Basic Energy Sciences of DOE.


KJ 10 Heat Capacity and Disorder in ScDx.* MARTIN MOSS, SANDIA Lab. -- Excess heat capacity in ScDx (x = 0.1-1.8) in the range 298-1000 K is greatest for x = 1. This can be explained by a disorder model which has been applied to cation-disordered phases in which a larger number of sites than mobile species leads to a configurational contribution to the entropy. It is assumed that high-energy interstitial sites are created by the introduction of deuterium, the occupation of the sites being temperature dependent. A two-level model for site energies leads to maxima in the entropy and heat capacity for mid-range values of x.

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** A U.S. DOE facility.


KJ 11 Evidence for Ordered Octahedral Protons Around Dilute Er in YH3.** R. V. L. Venturini, SANDIA Lab. -- We present evidence for ordered arrangements of octahedral protons around dilute Er ions in YH3 using electron spin resonance (ESR) of the Er in powdered hydride samples. When the hydrogen to metal ratio x is less than 2, we observe an isotropic ESR signal plus two distinct uniaxial resonances. The isotropic signal arises from an Er ion with eight nearest-neighbor tetrahedral protons (cubic site symmetry), and the uniaxial resonances correspond to Er ions with either one or two additional next-nearest-neighbor octahedral protons. A sample of YH3.4Er shows a new ESR signal from a site with biaxial symmetry (three unique axes) plus the isotropic signal from Er in a cubic site, but not the uniaxial site resonances just discussed. We have tentatively identified the biaxial Er site as the mer-X3 structure recently reported for stoichiometric PrD3. In this structure all eight tetrahedral proton sites are filled, and there are three ordered octahedral protons.

*Supported by the U.S. Department of Energy under Contract AT-(29-1)-796.

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KJ 12 Proton Distribution in Vicinity of a Rare Earth Impurity in a Hydride.** P. M. Richards, SANDIA Lab. -- Recent ESR and earlier Mössbauer studies of dilute Er

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