This paper showed the influence of interstitial hydrogen on the electronic states of palladium and nickel metals for various hydrogen concentrations. New electronic states are induced by the hydrogen. If these states are low, they are filled by electrons, which leads to stability of the hydride. The number and position of these states are given by the calculations and lead to nonrigid band behavior. Densities of states and electronic specific heat coefficients are also calculated for comparison. [The SC® indicates that this paper has been cited in over 225 publications.]

February 26, 1988

In 1969 Dick Heckman of Sandia's materials development organization introduced me to the area of metal hydrides with its dichotomous proton and anion models. The former model hypothesized that when hydrogen is incorporated into a metal it appears to lose its electron to fill the metal states (protonic), while in the latter model it apparently accepts an electron from the host (anionic). There was separate evidence for each viewpoint. This problem appealed to me as one in which the one-electron band theory of solid-state physics could provide some definitive answers. This paper was the fourth in a series applying this theory to various rare-earth and transition-metal hydrides.1,2

The paper was prepared for the International Meeting on Hydrides in Metals that was held in Jülich, Federal Republic of Germany, in March 1972, and it dealt with the classic, venerable system of palladium-hydrogen, and, for contrast, nickel-hydrogen. This was my first foreign meeting and represented my coming of age in "hydride land" with all its tribal taboos, high priests, and shibboleths. I chose the Berichte der Bunse Gesellschaft für Physikalische Chemie because it was the one in which the proceedings would be published. As it turned out, only the invited plenary papers along with the contributed abstracts were to be published as the conference proceedings. This paper, naively having been submitted earlier, preceded the conference publication.

The ideas expressed in this paper were confirmed by experimental work by Dean E. Eastman and J.K. Cashin and led to the writing of a Physical Review Letters paper3 with Eastman in my hotel room at the March 1971 meeting of the American Physical Society in Cleveland. Calculations on these and other hydride systems were able to show which electron states were filled in each case and to reconcile the two disparate models. My later refinement of these ideas led me to the concept of a minimum hydrogen-hydrogen distance of 2.10 angstroms in metal hydride systems. Experimental and theoretical work in Germany, France, Israel, the USSR, and the US (at Ames, Argonne National Laboratory, Harvard, IBM, the Naval Research Laboratory, and other laboratories) has subsequently shown the appropriateness of such calculations for hydride systems.4

The numerous citations to this work reflect, I believe, that it was the right stuff, at the right time, and in the right place. Shortly before this meeting, superconductivity had been discovered in palladium hydride by T. Skoskiewicz,5 and his presentation created considerable excitement for those days. This discovery was followed by the observation of an inverse isotope effect where palladium deuteride had a higher superconducting transition temperature than the hydride, contrary to conventional thinking. These results made such calculations all the more relevant. This meeting and subsequent symposia on hydrides in metals and metal hydrides were eminently successful in that they brought together chemists, metallurgists, chemical engineers, and physicists (now called materials scientists), all working on aspects of a common problem. With growth and maturity in the field, the forum for hydrides has fallen to the Journal of the Less-Common Metals.6,7 I am now studying boron and boron compounds and have found many technical, professional, and sociological parallels—plus ça change, plus c'est la même chose.

2. ———. Metal hydrides—structure and band structure. J. Quantum Chem. 5:499-509, 1971. (Cited 100 times.)

1Supported by the US DOE under Contract DE-AC-04-0P00789

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