

**NUCLEAR MAGNETIC RESONANCE STUDIES ON  
HYDRIDES OF SOME INTERMETALLIC COMPOUNDS**

**DISSERTATION SUBMITTED FOR THE DEGREE OF  
DOCTOR OF PHILOSOPHY (SCIENCE)  
OF THE  
UNIVERSITY OF CALCUTTA**

**BILWADAL BANDYOPADHYAY  
SAHA INSTITUTE OF NUCLEAR PHYSICS  
CALCUTTA  
OCTOBER, 1991**

# INDEX

## CHAPTER 1 INTRODUCTION

	PAGE
1.1. <i>Introduction to metal hydrides</i>	1
1.1.1. <i>Solution of hydrogen in metals</i>	3
1.1.1.1. <i>Solid solution and the hydride</i>	5
1.1.2. <i>Enthalpy and entropy of metal-hydrogen reaction</i>	6
1.1.3. <i>Location of H atom in metals</i>	9
1.1.4. <i>Diffusion of hydrogen in metals</i>	10
1.1.5. <i>Effect of hydrogen on electrical and magnetic properties of metals</i>	11
1.1.5.1. <i>Review on some experimental observations</i>	13
1.2. <i>Background and objective of present work</i>	17

## CHAPTER 2 THEORETICAL BACKGROUND

2.1. <i>The phenomenon of nuclear magnetic resonance (NMR)</i>	22
2.1.1. <i>Broadening of resonance lines</i>	24
2.1.1.1. <i>Dipolar broadening</i>	24
2.1.1.2. <i>Broadening due to electron-nuclear interaction</i>	28
2.1.2. <i>Nuclear magnetic relaxation in metal-hydrogen systems</i>	32
2.1.2.1. <i>Effect of random isotropic motion of spins on nuclear magnetic relaxation</i>	34
2.1.2.2. <i>Crystal lattice dependent models of atomic diffusion in solids</i>	42
2.1.2.3. <i>Effect of electron-nuclear interaction on nuclear spin-lattice relaxation</i>	49
2.2. <i>A brief review of results obtained from NMR experiments on metal hydrides</i>	59
2.2.1. <i>Structural information</i>	59
2.2.2. <i>Hydrogen diffusion and electronic structure</i>	61

CHAPTER 3      EXPERIMENTAL

	PAGE
3.1. <i>Preparation of samples</i>	65
3.1.1. <i>Development of a gas-doping apparatus</i>	65
3.1.2. <i>Preparation of hydrides</i>	69
3.1.2.1. <i>Pressure-composition (p-c) isotherms</i>	70
(a) <i>YNiAl-H</i> and (b) <i>CeNiAl-H</i>	
3.1.3. <i>X-ray studies on prepared hydrides</i>	71
3.2. <i>Experimental techniques</i>	73
3.2.1. <i>Pulse width and frequency distribution</i>	75
3.2.2. <i>Dead-time and spin-echo</i>	76
3.2.3. <i>The inversion-recovery method of</i>	79
determination of $T_1$	
3.3. <i>Instruments</i>	81

CHAPTER 4      RESULTS AND DISCUSSION

4.1. <i>Results of magnetic susceptibility measurements</i>	82
4.1.1. <i>Measurements on parent compounds</i>	82
4.1.2. <i>Measurements on hydrides</i>	84
4.1.3. <i>Summarizing remarks</i>	86
4.2. <i>Results of nuclear magnetic resonance</i>	88
(NMR) studies	
4.2.1. <i>ZrNiAlH<sub>x</sub></i>	88
4.2.2. <i>YNiAlH<sub>x</sub></i>	89
4.2.2.1. <i>CW measurements</i>	89
4.2.2.2. <i>Effect of diffusion on linewidth</i>	91
4.2.2.3. <i>Measurements of <sup>1</sup>H spin-lattice relaxation time</i>	93
4.2.3. <i>CeNiAlH<sub>x</sub></i>	97
4.2.3.1. <i>Field dependence of linewidth</i>	99
4.2.3.2. <i>Temperature dependence of linewidth</i>	101
4.2.3.3. <i>Results of <sup>1</sup>H spin-lattice relaxation time</i>	104
measurements	
4.2.4. <i>Conclusion</i>	112

APPENDICES

REFERENCES