PREFACE

Energy is essential for our life activities. It is a predominant factor in the development of mankind. With the rapid increase in global population along with the growing demand in the developing countries in order to improve their living standards, it is understood that there will be a great demand for energy. We have many energy resources which are available on earth. At present coal, petroleum products and nuclear fuel assist our energy needs. The petroleum products will not be available for long time because of the population and the usage. Tapping energy from nuclear sources is not only a costly process but also a hazardous job which many countries may not be able to afford. The energy crisis can be overcome by the naturally available solar power. The solar energy is a gift of nature as alternate energy source which is not only cheap, efficient and safe but can also sustain for a very long time. Solar energy evolves as a dependable energy source without the aid of a highly technical and specialised nature for its wide spread utilisation. It offers a vision of hope and a plan to begin the long journey towards energy independence and global healings. The best pollution free alternative to energy source is the hydrogen fuel in which hydrogen and oxygen combine to produce energy and steam, as the only by-product. Hydrogen is produced through solar powered electrolysis process (the separation of water into hydrogen and oxygen) and burnt as a fuel or used in a fuel cell to produce electricity.
Hydrogen storage is an important phenomenon because of its relevance to the energy economy of the future. Since hydrogen is a versatile fuel and can be readily generated and converted into other forms of energy – to store hydrogen is to store energy. Hydrogen has the highest energy density per unit weight and has number of uses ranging from internal combustion engines to hydrogen fuel cells. The important problem associated with hydrogen when used as a fuel, is its economic and convenient storage. Hydrogen isotopes diffuse fast in alloys. Metals and alloys would be used to store hydrogen safely. Much hydrogen can be easily absorbed and later, by a slight change of parameters, recovered. The metals or alloys used for hydrogen storage should fulfill the following requirements. They should be capable of storing large quantities of hydrogen and have reaction kinetics satisfying the charge/discharge requirements of the system and have low cost.

In hydrogen diffusion, it is necessary to have knowledge about diffusion parameters in order to choose a better element or compound to store hydrogen. With this concept in mind, the researcher undertook this theoretical work entitled “LATTICE DYNAMICAL INVESTIGATION ON SOME HYDROGEN STORAGE MATERIALS” under the guidance of Dr. N. Lawrence, Reader in Physics, Department of Physics, St. Joseph’s College (Autonomous), Tiruchirappalli during the period from January 2002 to December 2006.
The thesis is divided into seven chapters. The content of the various chapters are summarised below:

Chapter I gives an outline about the research work which describes the availability of various energy sources and the need of hydrogen storage, the suitability of solid metal hydrides for hydrogen storage and the requirements for a metal/alloy to be a good hydrogen storage media.

Chapter II presents a review of the diffusion of hydrogen isotopes in metals and alloys. The experimental techniques and theoretical models to calculate the diffusion parameters are described in detail. The experimental and theoretical results are summarized for important storage media which are available in the literature.

In Chapter III, the theoretical model used in the calculations is explained. The Born-von Karman formalism for the calculation of phonon dispersion, the Green’s function technique and scattering matrix formalism for the calculation of Mean Square Displacement (MSD) values and reaction coordinates for the calculation of diffusion parameters have been described.

Chapter IV deals with the lattice dynamical investigation of Pd-H system. The phonon frequency distribution of Palladium system and the mean square displacement of Pd atoms surrounding the hydrogen atom are calculated using Green’s function technique and scattering matrix formalism. The calculated MSD values in the H defect situation are found to be less than that of the host crystal.
In chapter V, the calculated diffusion parameters of hydrogen and deuterium in Pd$_{0.95}$Ru$_{0.05}$ and Pd$_{0.90}$Ru$_{0.10}$ alloys are reported. The MSD values of Pd$_{0.95}$Ru$_{0.05}$ and Pd$_{0.90}$Ru$_{0.10}$ alloys surrounding the hydrogen atom are calculated using Green's function technique and scattering matrix formalism. The diffusion co-efficient of hydrogen isotopes in Pd$_{0.95}$Ru$_{0.05}$ and Pd$_{0.90}$Ru$_{0.10}$ alloys are compared with the experimental values and are found to be in good agreement. The calculated values have been compared with the available experimental and other theoretical data for similar systems.

Chapter VI presents the results of lattice dynamical study on Ni$_{0.55}$Pd$_{0.45}$ and Fe$_{0.72}$Pd$_{0.28}$ systems and the calculated results of the MSD, diffusion co-efficient and activation energy at different temperatures and pressures are given. The theoretically calculated values are compared with the existing experimental and other theoretical results.

In Chapter VII, the results of all the systems of the study are consolidated, compared and their relevance for hydrogen storage have been discussed.

A major part of the results presented in the thesis has been published in journals / communicated to journals.