Designing Mg-Li Binary Alloys for Hydrogen Storage Applications

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Project Under the guidance of
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Motivation of the Project

The main aim behind this project is to design a materials made up of Mg-Li Binary alloy which would be used out for the storage of Hydrogen gas and we would look upon its various applications in real aspects.

Various Ideations and their Proposed Solutions

(A.) Importance of Hydrogen storage at the Industrial Level

(B.) Study of Materials used out presently for Hydrogen storage along with their special characteristics.

(C.) Why Mg-Li alloys as Hydrogen Storage Material.

(D.) Theoretical Predictions of different Mg-Li alloys for Hydrogenation and De Hydrogenation Kinetics

(E.) Classification based on crystal structure, Role of vacancies and interstitials to improve the hydrogen storage.

(F.)Explaining hydrogenation and dehydrogenation process with help of flowcharts on Mg based alloys.

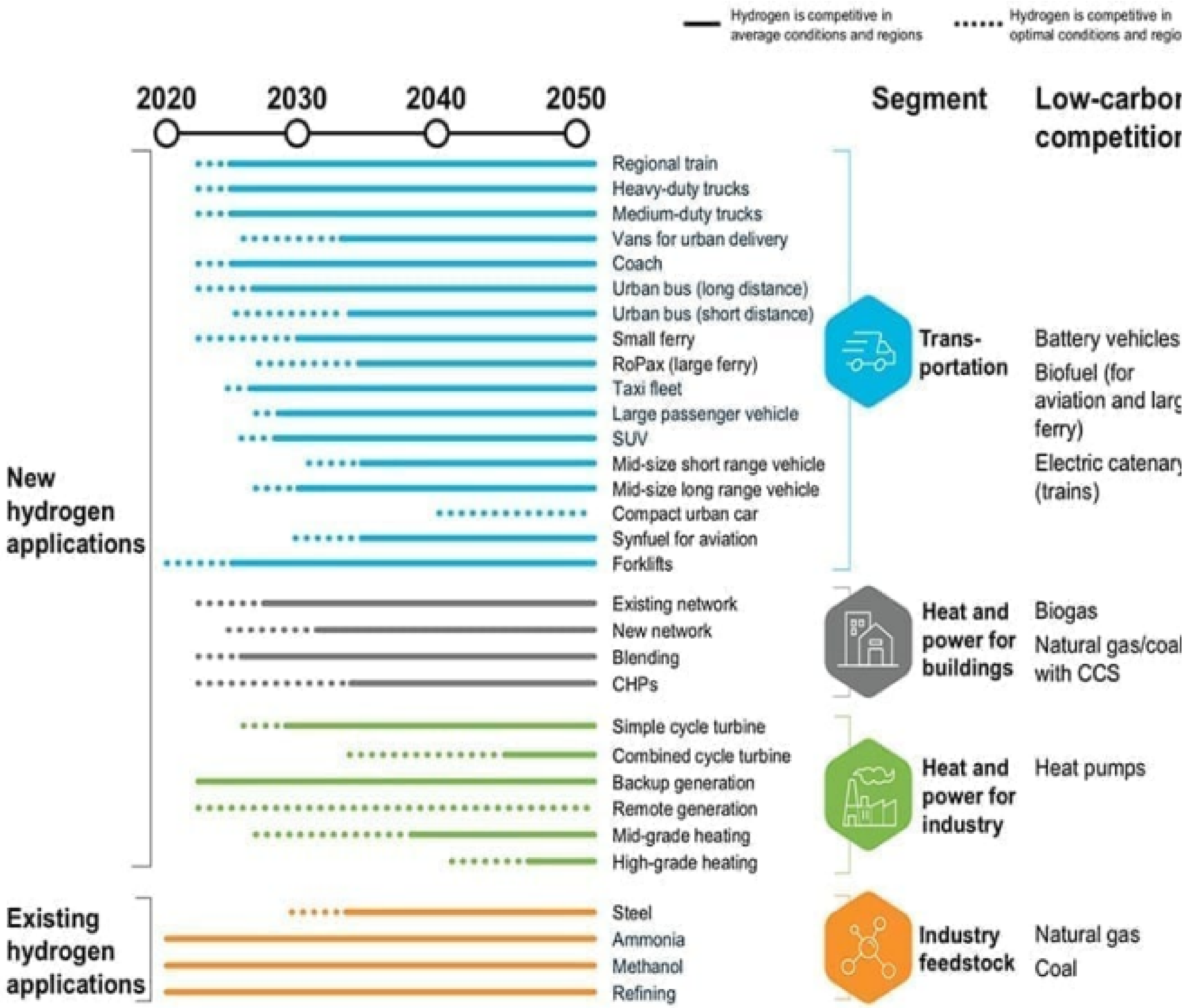
(G.) Macrostructure of Magnesium AZ31 alloy

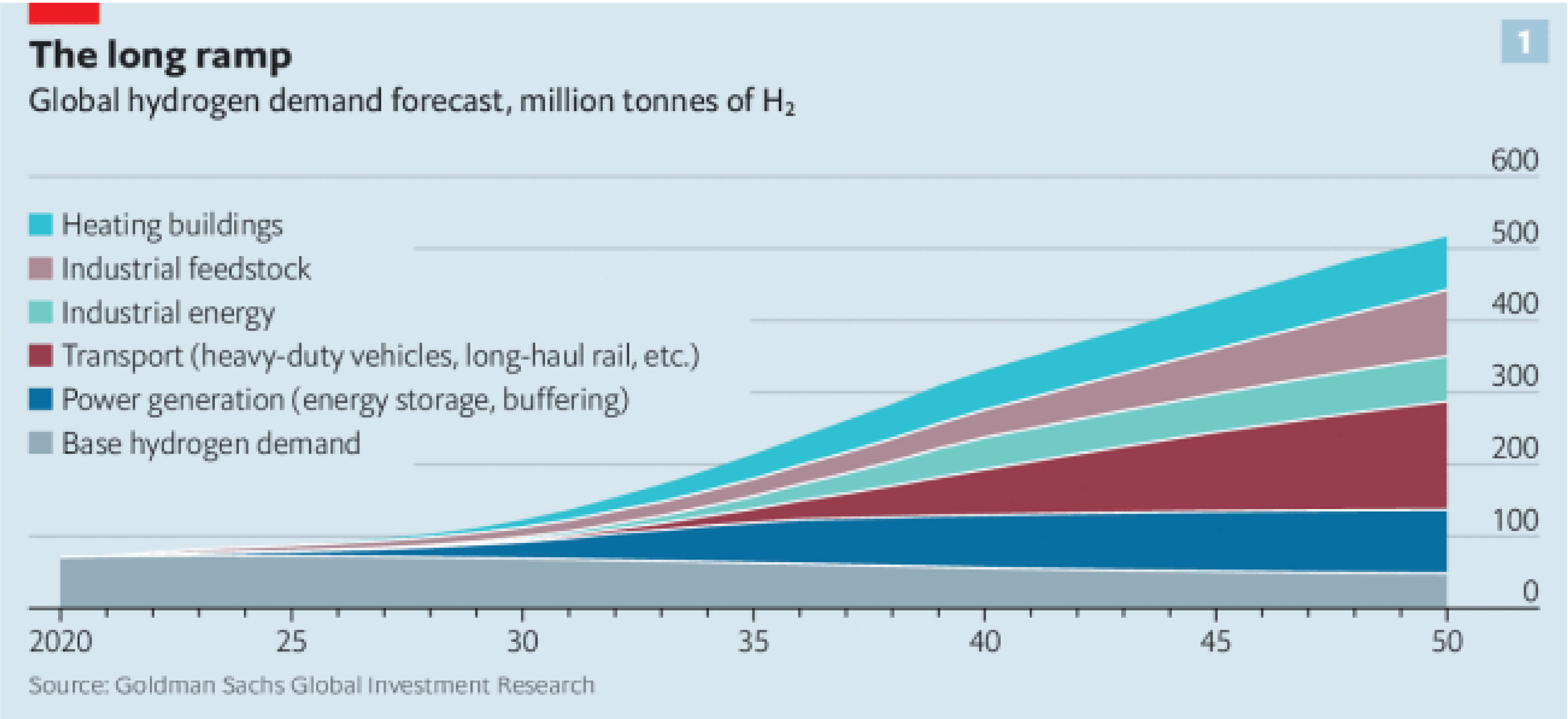
Importance of Hydrogen Storage at Industrial Level

The rising population and increasing demand for energy supply urged us to explore more sustainable energy resources. The reduction of fossil fuel dependency in vehicles is key to reducing greenhouse emissions.

As a fuel of choice it is light weight, contains high energy density and its combustion emits no harmful chemical by-products. Moreover, hydrogen is considered as a green energy, because it can be generated from renewable sources and is non-polluting .

Some of the applications of Hydrogen at Industrial Level are as follow:


Hydrogen is competitive in average conditions and regions
Hydrogen is competitive in optimal conditions and regio
2020
2030
2040
2050
Segment
Low-carbo
competitio
New hydrogen applications
Regional train
Heavy-duty trucks
Medium-duty trucks
Vans for urban delivery
Coach
Urban bus (long distance)
Urban bus (short distance)
Small ferry
RoPax (large ferry)
Taxi fleet
Large passenger vehicle
SUV
Mid-size short range vehicle
Mid-size long range vehicle
Compact urban car
Synfuel for aviation
Forklifts
Trans-portation
Battery vehicles
Biofuel (for aviation and larg ferry)
Electric catenar (trains)
Existing network
New network
Blending
CHPs
Heat and power for buildings
Biogas
Natural gas/coal with CCS
Simple cycle turbine
Combined cycle turbine
Backup generation
Remote generation
Mid-grade heating
High-grade heating
Heat and power for industry
Heat pumps
Existing hydrogen applications
Steel
Ammonia
Methanol
Refining
Industry feedstock
Natural gas
Coal



The Economist

The goal of the stationary storage of hydrogen is generally either to minimize the cost of delivered hydrogen through the balancing of supply and demand or to use it for backup purposes. The demands of a particular application may have a substantial influence on the capital and operating costs of the storage .

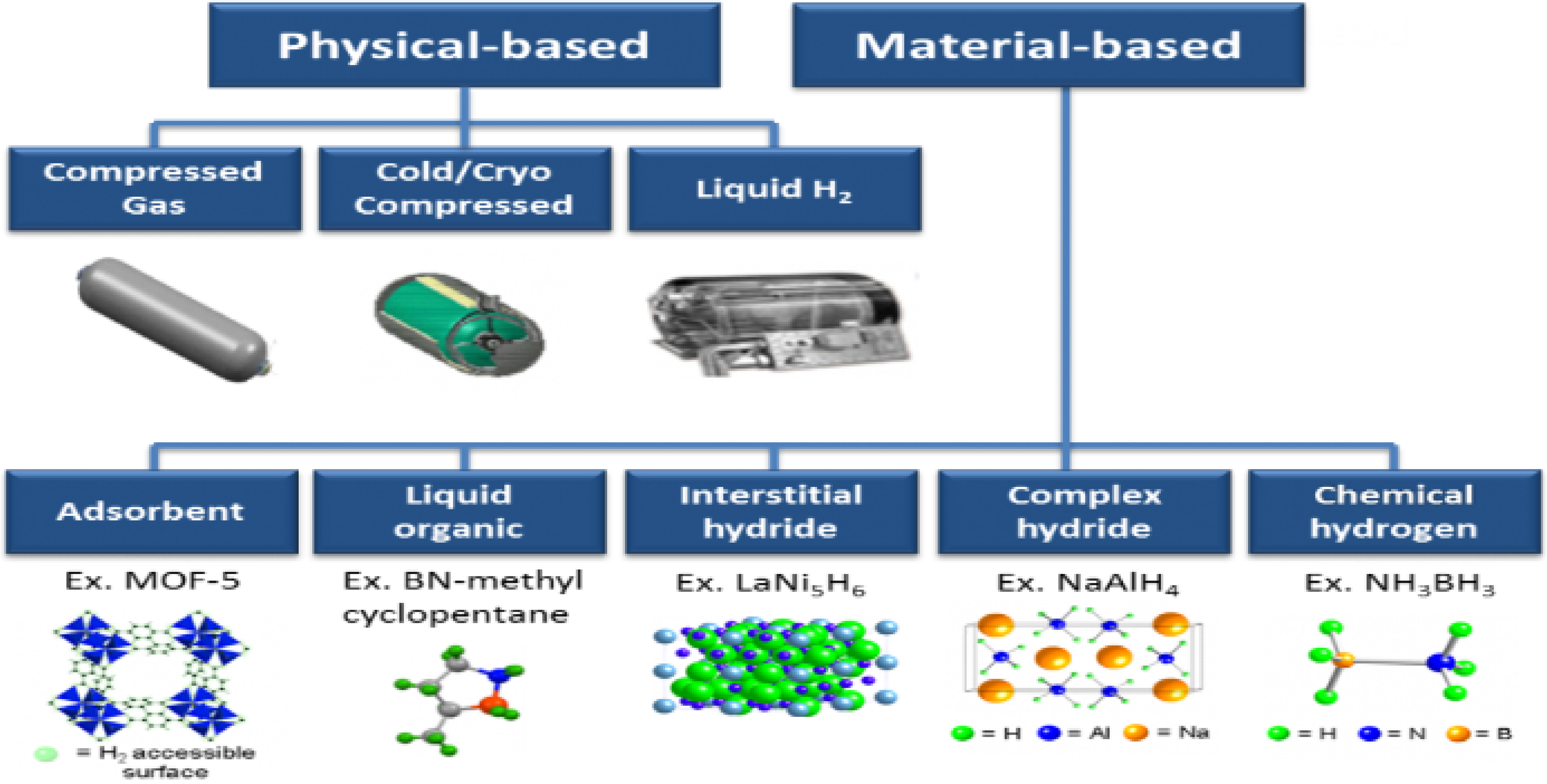
Materials which are being used in Hydrogen storage and their special characterstics

(a.) Recently, various kinds of materials have been studied, where the following properties are required:

1. High gravimetric and volumetric density of hydrogen.
2. Suitable thermodynamic properties, which are the reversible hydrogen sorption/desorption under moderate temperature and pressure.
3. Rapid kinetics.
4. Easy handling.
5. Abundant resources and low cost.

(b.) The hydrogen storage capacity of a material depends on the structure and the type of interaction with hydrogen. There are several new and novel materials available for hydrogen storage.

How is hydrogen stored?



Why Mg-Li alloys as Hydrogen Storage Material

(a.)Mg-Li alloys are a good option due to their abundance and availability as well as their extraordinary high gravimetric and volumetric storage densities.

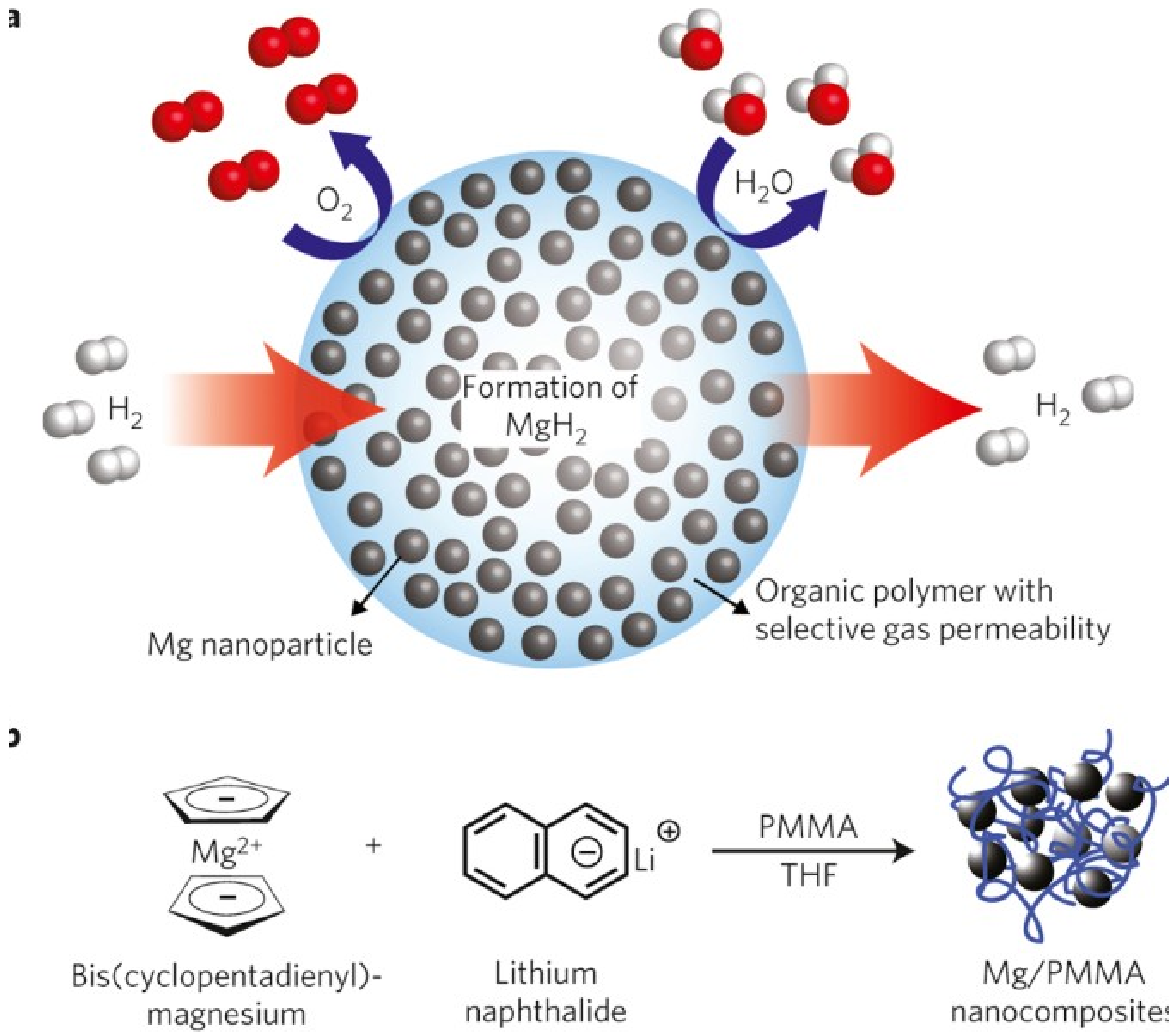
(b.) The occurrence of α-Mg(Li) and β-Li(Mg) phases in the Mg-Li binary system is characterized by the presence of ordered and disordered forms of magnesium, which may impact the hydrogenation characteristics of magnesium.

(c.) Hence study over the lithium level and it's impact over the storage was being done out.

(d.) Therefore, the hydrogenation properties of Mg-Li alloy modified by the addition of 4.0 wt.%, 7.5 wt.% and 15.0 wt.% lithium were studied and the observations were being observed out for each and every case .

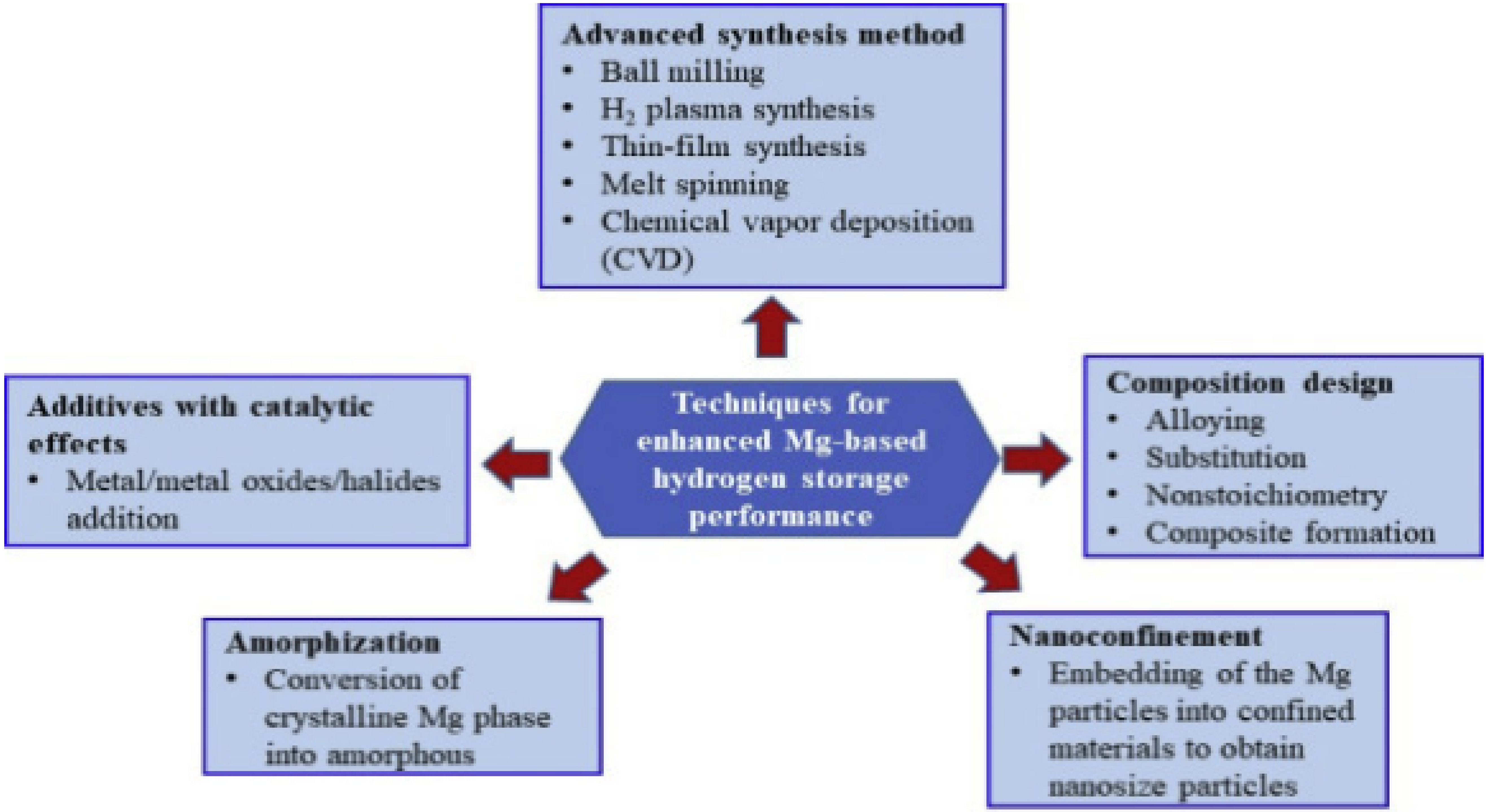
(e.) It was observed that, along with an increase in lithium content, the grinding conditions changed, which affected the morphology and particle size of the tested powders.

(f.) Magnesium hydride obtained as a result of the hydrogenation of this alloy modified with lithium (4.0 wt.%, 7.5 wt.% and 15.0 wt.%) was characterized by a high hydrogen desorption activation energy .

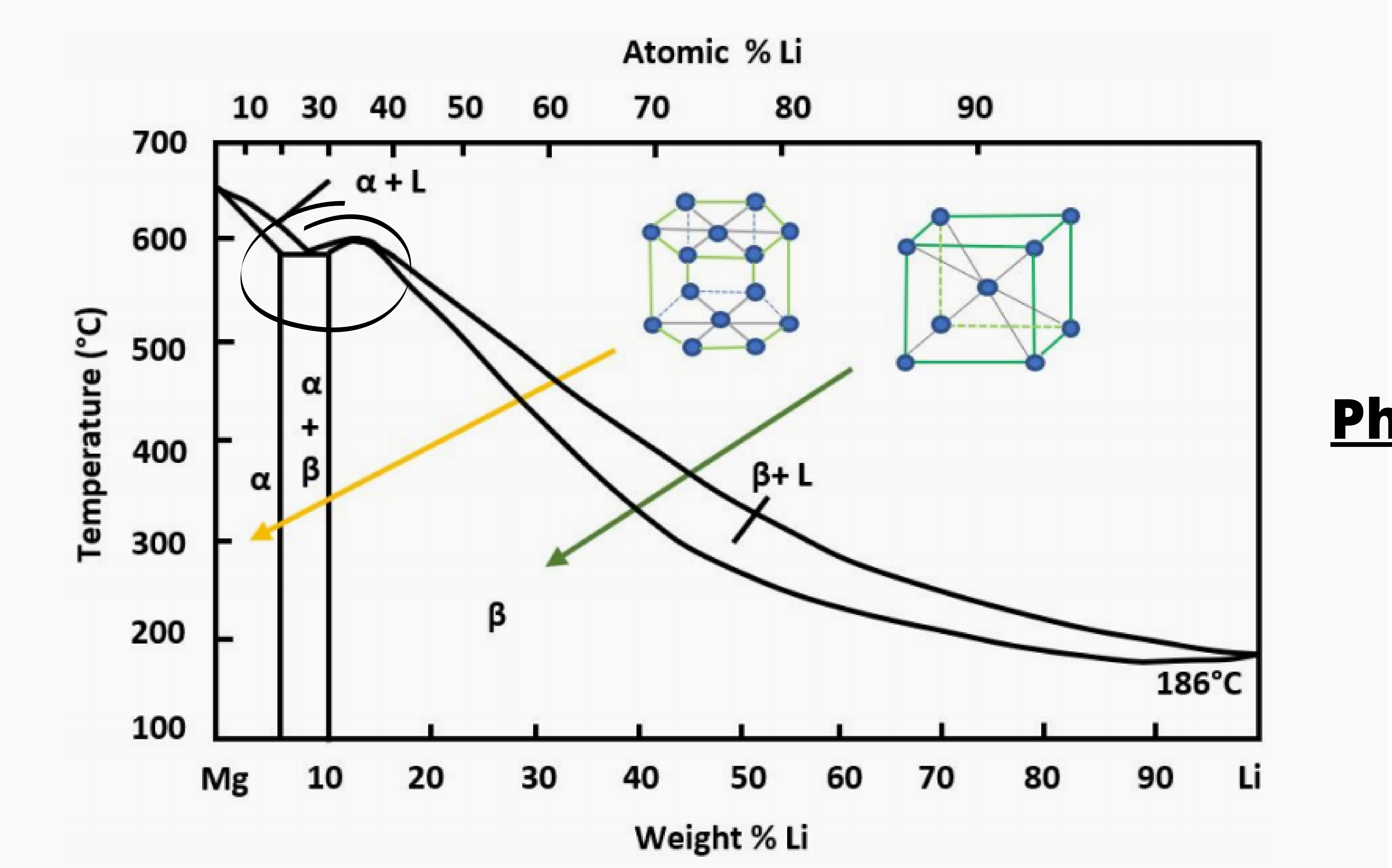


How Mg-Li alloys help in Hydrogen Storage

Techniques for enhanced Hydrogen Storage



Theoretical Predictions of different Mg-Li alloys for Hydrogenation and De-Hydrogenation Principles



Phase Diagram of Mg-Li based alloys

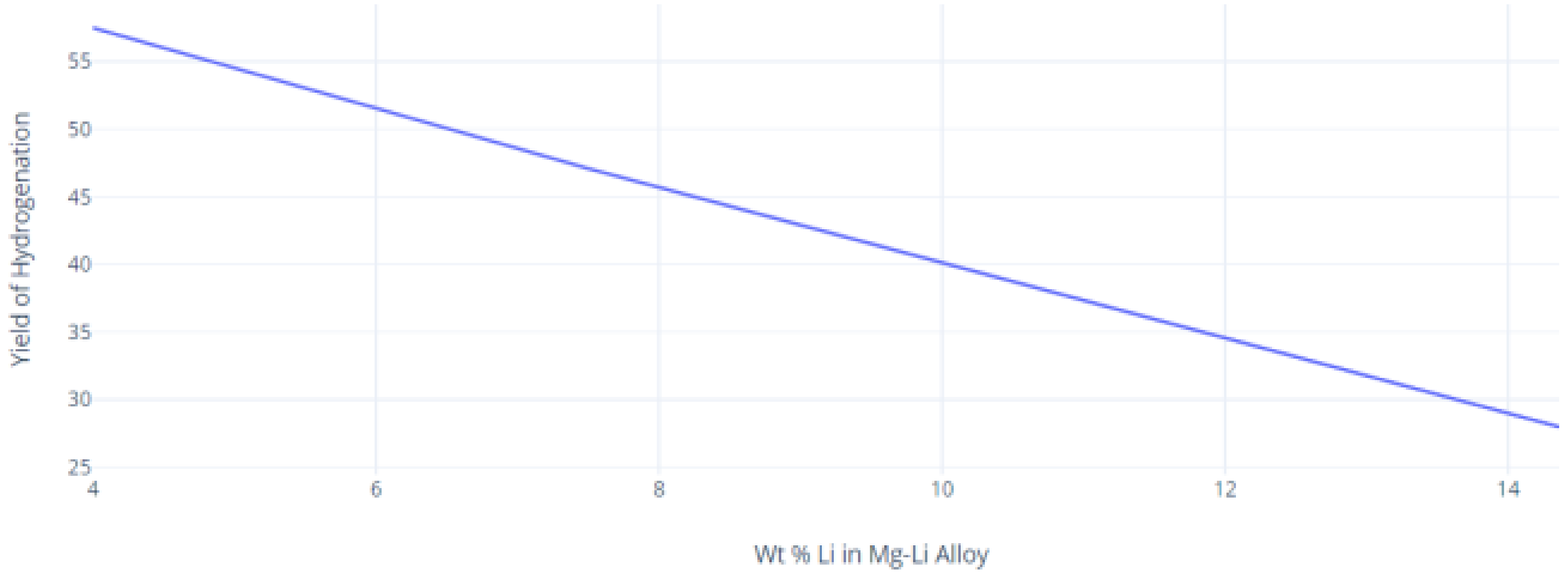
(a.) As a result of hydrogenation of a modified Mg-Li alloy, magnesium hydride was obtained. It was characterized by a high hydrogen content, with additions of 4.0 wt.%, 7.5 wt.%, and 15 wt.% lithium . There were activation energies of 250, 187, and 224 kJ/mol, respectively.

(b.)To determine the effect of the phase structure of the Mg-Li alloy on its hydrogenation properties,
alloys with different lithium contents of 4.0 wt.%, 7.5 wt.% and 15.0 wt.% were tested. The graphs and tests results are being taken out next.

Table 2. The hydrogenation properties of alloys with various lithium contents.

Sample	Theoretical Hydrogen Capacity in MgH_2 (wt.%)	Measured Hydrogen Capacity in MgH_2 (wt.%)	Yield of Mg Hydrogenation Reaction (%)
Mg 4.0 wt.% Li	7.3	4.2	57.5
Mg 7.5 wt.% Li	7.0	3.3	47.1
Mg 15.0 wt.% Li	6.5	1.7	26.2

To Depict Hydrogenation Capacity with the increase in Wt% of Li in Mg-Li Alloy



Problems and Solutions of different Mg-Li alloys for Hydrogenation and De Hydrogenation Kinetics Principles

(a) Materials for hydrogen storage should be lightweight. Mg-Li compounds have this potential. This scientific topic has so been pursued for a long time. The low (de)hydrogenation kinetics of magnesium alloys looked to be a major disadvantage.

(b.) Fluorite-based magnesium alloys alloyed with scandium have been examined electrochemically in compositions ranging from 50% to 100%. The favourable discharge kinetics were preserved up to 80% magnesium.

(c.) The improved (de)hydriding kinetics over pure magnesium is due to scandium hydride's open fluorite structure rather than the compact rutile structure of ordinary magnesium hydrides.

(d) Recently, attempts have been undertaken to create cheaper alternatives to scandium. Scandium hydride is a dihydride of titanium and lithium, which has the same fluorite structure. The discharge (dehydrogenation) kinetics of Mg80Ti20 and Mg80Li20 thin film electrodes were equivalent to pure magnesium hydride (MgH2).

(e.) A closer look at the Mg–Li system revealed that, like the Mg–Sc system, the hydrogen storage capacity was composition dependent, with a maximum around 80% magnesium.

(f.) While challenges like deterioration and material expense still need to be addressed, this new family of magnesium materials may be useful for applications that need gas phase storage of hydrogen.

Classification based on crystal structure, Role of vacancies and interstitials to improve the hydrogen storage.

(a.) When the concentration of hydrogen in the alloy comes to a certain limit, metal hydrides are formed. As a result, hydrogen occupies certain sites among the metal lattices.

(b.) Properties of hydrogen storage in an alloy are determined by the interaction of hydrogen with metal atoms at the interstitial site, and hence, the hydrogen storage characteristics depend largely upon the crystal structure of the alloy.

(c.) Up to now, a number of hydrogen-storing alloys have been developed, and they may be classified into five groups shown , based on the crystal structure of alloy and the similarity of hydriding characteristics .

Type	Alloy	Crystal structure
A_2B	Mg_2Ni	(P6222)
	Mg_2Cu	(Fddd)
AB	TiFe	B2(CsCl)
	TiCo	B2 (CsCl)
	ZrCo	B2 (CsCl)
	ZrNi	(CrB)
AB_2	$TiCr_{1.8}$	C15
		C14
	$TiMn_{1.5}$	C14
	$ZrCr_2$	C15
		C14
AB_5	$CaNi_5$	($CaCu_5$)
Solid Solution	Ti-V	BCC
	V-Nb	BCC

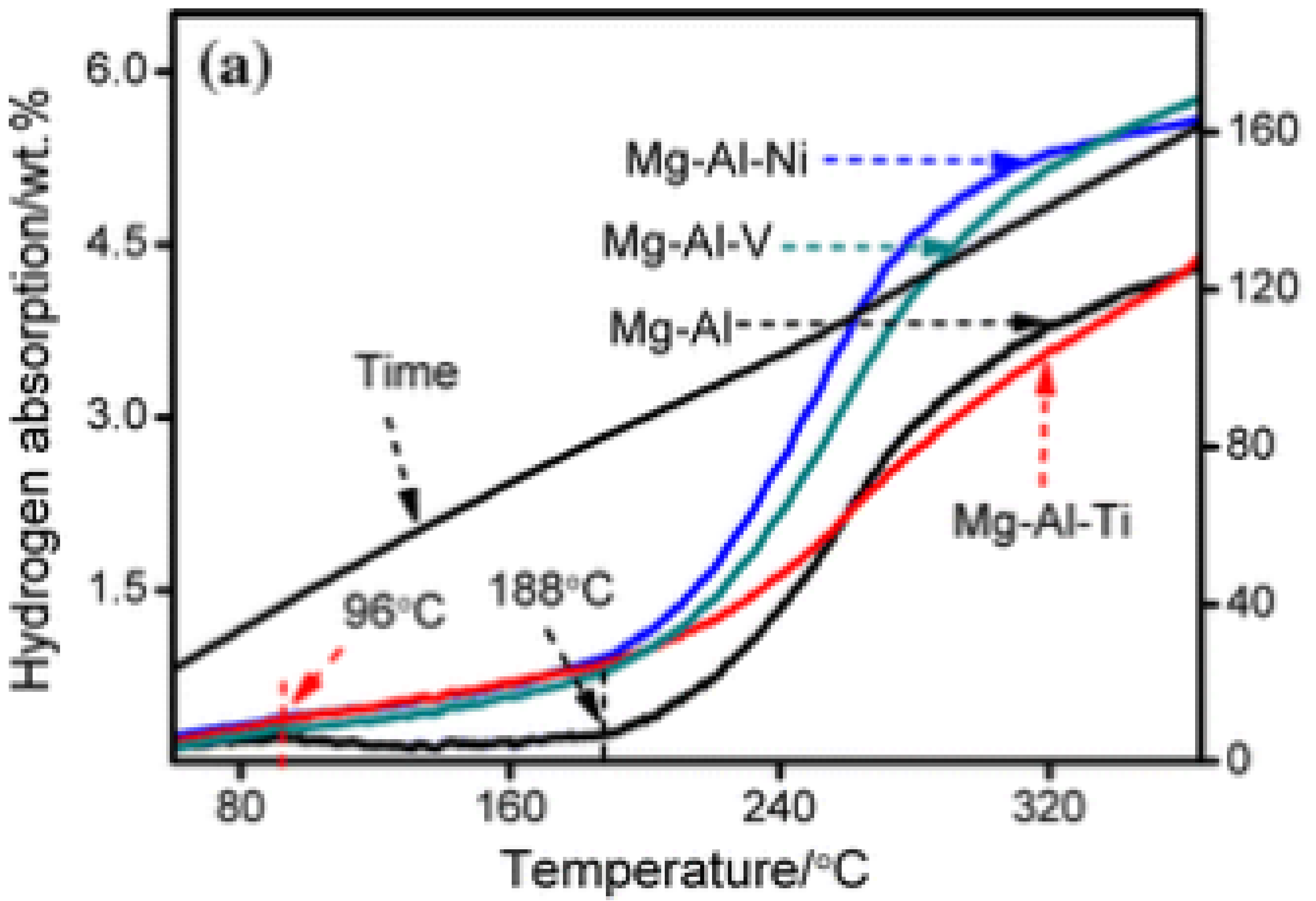
Different types of Alloy along with their possible crystal structure

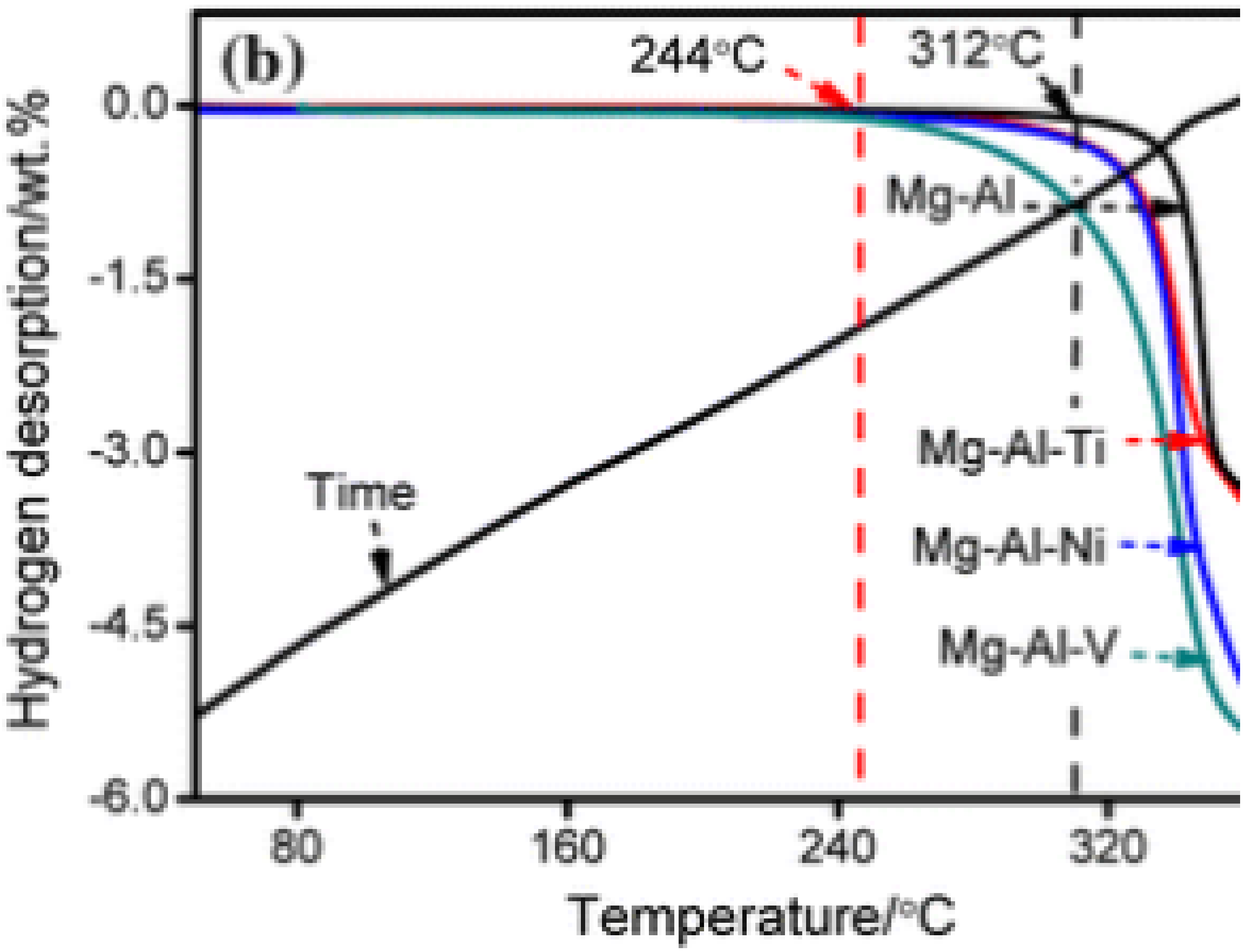
(d.) We found that a number of transition-metal impurities and vacancies are effective in shifting the Fermi level as well increasing the Hydrogen storage capacity. Different impurities in different configurations, however, produce shifts of different magnitudes (or do not shift the Fermi level at all)

(g.). Among the possible positions, the impurities can be nominally on the Li, and Mg sites, and at interstitial sites. For each type of substitutional or interstitial impurity, calculations can be carried out in various configurations to be sure that the lowest-energy configurations are obtained.

(h.) Significant effort has to be devoted to make sure that the global minimum is identified to get the most stable system for the Hydrogen Storage.

Explaining hydrogenation and dehydrogenation process with help of graph for Mg based Alloys





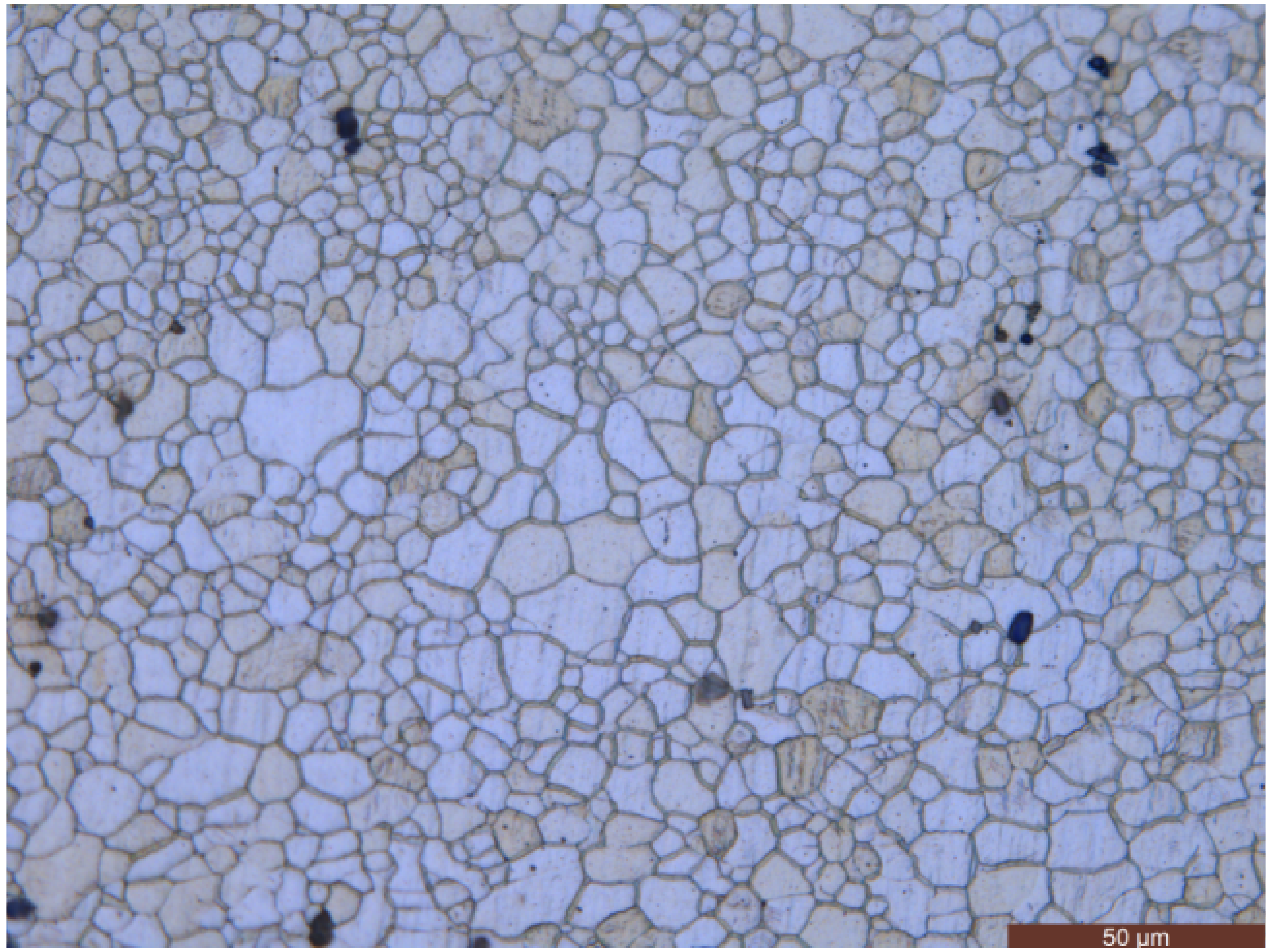
Practical Aspects of the Project and Viewing out the Macro-structures of Mg AZ31 for Hydrogen Storage

(1.) Paper Polishing: 400-2000 grit emery paper was being used out and this will generate a reflective finish on most common non-hardened metals and is the preferred technique for polishing metals prior to Lapping.

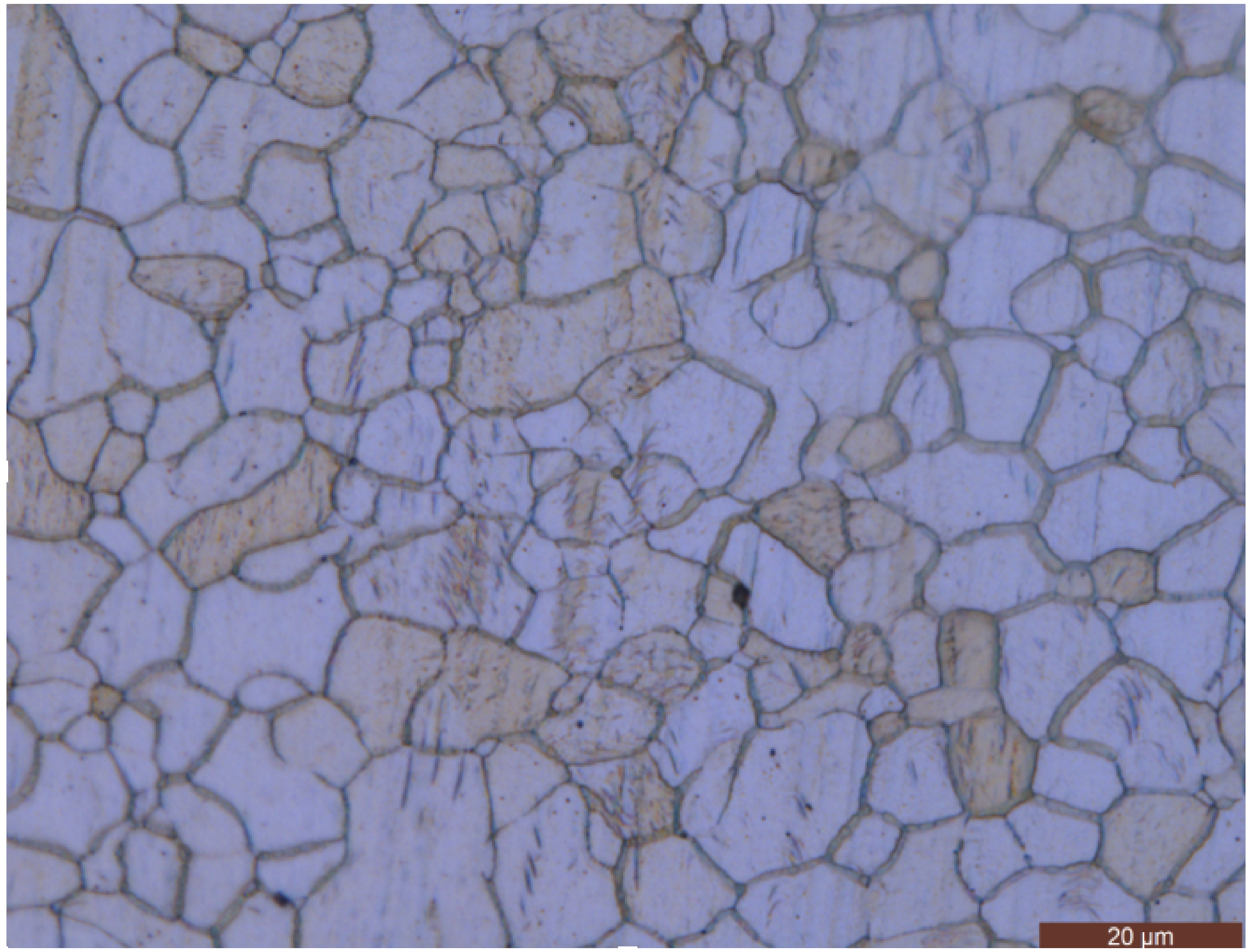
2.) Cloth Lapping: Lapping is a machining process in which two surfaces are rubbed together with an abrasive between them, by hand movement or using a machine. In this whole process Kerosene was being used out during the time of lapping.

3.) Etching: Etching is used to reveal the macrostructure of the metal through selective chemical attack. It gives out the grain boundaries which have higher energy than grains which corrodes out and gives us the macrostructures.

4.) The given extracted image of the Magnesium AZ31 macrostructures obtained during the practical work are being attached



Extracted Macrostructures of Mg AZ31 at 50 µm



Extracted Macrostructures of Mg AZ31 at 20 µm

Bibliography

I want to thanks and mention the following links and papers which had helped me to gain out some knowledge for this project . Without the help of Dr. Saurabh Sanjay Nene sir , this report would have been an indefinite task for me.

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Thank You