

## **Methods for Forming Hydrogen Clusters**

### **TECHNICAL AREA:**

*A metal alloy composite particle material that reversibly reacts with gaseous hydrogen and/or its isotopes by absorption and desorption.*

### **BACKGROUND:**

*A gas-loaded heat generator capable of producing a thermal energy by interaction between one or more isotopes of hydrogen and a plurality of metallic micro-structures is reported. The metallic micro-structure as a plurality of micro-nano particle could be a base for reversible reactions of absorption and desorption.*

### **EXISTING TECHNOLOGIES:**

*Most of metallic materials that reversibly react with gaseous hydrogen and/or its isotopes are in alloys or intermetallic compounds, usually in a combination of metals with higher hydrogen affinity and with non-hydrogen affinity. These materials could be pulverized or filmed to maximize gas contact due to its increased surface area. The absorbed hydrogen and/or its isotopes forms beta phase hydride inside of metal lattice.*

### **PROBLEMS WITH EXISTING TECHNOLOGIES:**

*The tailored metallic alloy or compounds absorb and desorb gaseous hydrogen and/or its isotopes into its lattice as a single atom and forms a chemically stable beta phase hydride or deuteride therefore the whole bulk has a limited capacity of hydrogen and/or its isotopes.*

### **SUMMARY OF THE PROPOSED SOLUTIONS AND THE ADVANTAGES THE PROPOSED SOLUTIONS PROVIDE:**

*The basic idea is a method to form not a single but a multiple and therefore dense hydrogen and/or its isotopes into vacancy including defect and*

*dislocation inside of the metallic or intermetallic compound or metallic composite material bulk using the hydrogen and/or its isotopes atom mobility as an alpha phase of solid solution and therefore to increase the probability of hydrogen and/or its isotopes atom trapped into the vacancy in order to maximize the amount of overall hydrogen and/or its isotopes absorption.*

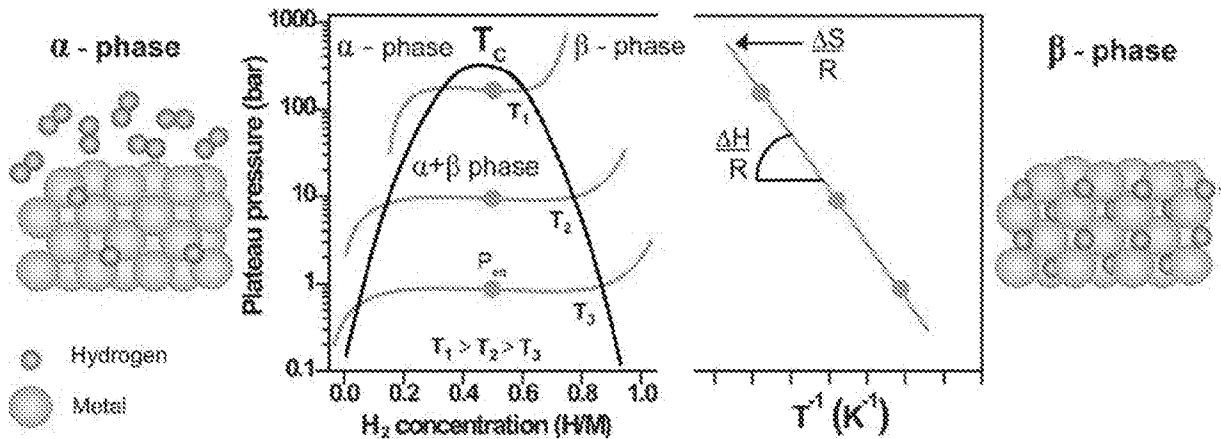
## **DETAILED DESCRIPTIONS OF THE PROPOSED SOLUTION AND FIGURES:**

### **1. Principle of the cluster formation**

*The thermodynamic aspects of metal hydride formation are examined through pressure-composition isotherms (Fig. 1). At small hydrogen to metal ratios ( $H/M \leq 0.1$ ) below a certain pressure,  $H_2$  is dissolved in the metal as a solid solution  $\alpha$  phase. As the  $H_2$  concentration increases and pressure rises, the stable metal hydride  $\beta$  phase nucleates and grows. While the two phases co-exist, a plateau at constant pressure is observed, the width of which determines the hydrogen storage capacity of the material. The two-phase region ends at a critical temperature ( $T_C$ ) beyond which the transition from  $\alpha$  to  $\beta$  phase is continuous. The plateau pressure correlates to the change in enthalpy ( $\Delta H$ ) and entropy ( $\Delta S$ ) as a function of temperature by the Van't Hoff equation;*

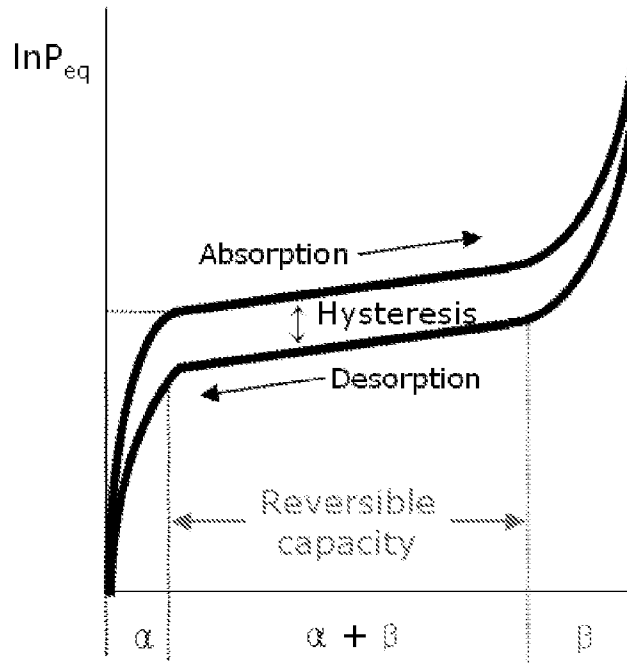
$$\ln\left(\frac{P_{eq}}{P_o}\right) = \frac{\Delta H}{RT} - \frac{\Delta S}{R}, \text{ while enthalpy determines the strength of the metal-}$$

*hydrogen bond, entropy corresponds to the change from molecular hydrogen to hydrogen in the hydride phase.*



[Fig. 1] Pressure concentration Isotherm and van't Hoff diagram

The absorption process from the gaseous form of hydrogen and/or its isotopes to the metallic form of same is as follows; 1) Physisorption of gaseous hydrogen and/or its isotopes by van der Waals force → 2) chemisorption via H-H dissociation of exothermic reaction → 3) H atom solvation to form alpha phase solid solution of endothermic reaction → 4) chemical reaction to form beta phase hydride of exothermic reaction. The desorption process follows the same but reversed procedure. This reversible process however in reality it always comes with hysteresis which is irreversibility of energy balance between absorption exotherm and desorption endotherm that is characterized by the pressure-concentration isotherm shown in Fig.2.

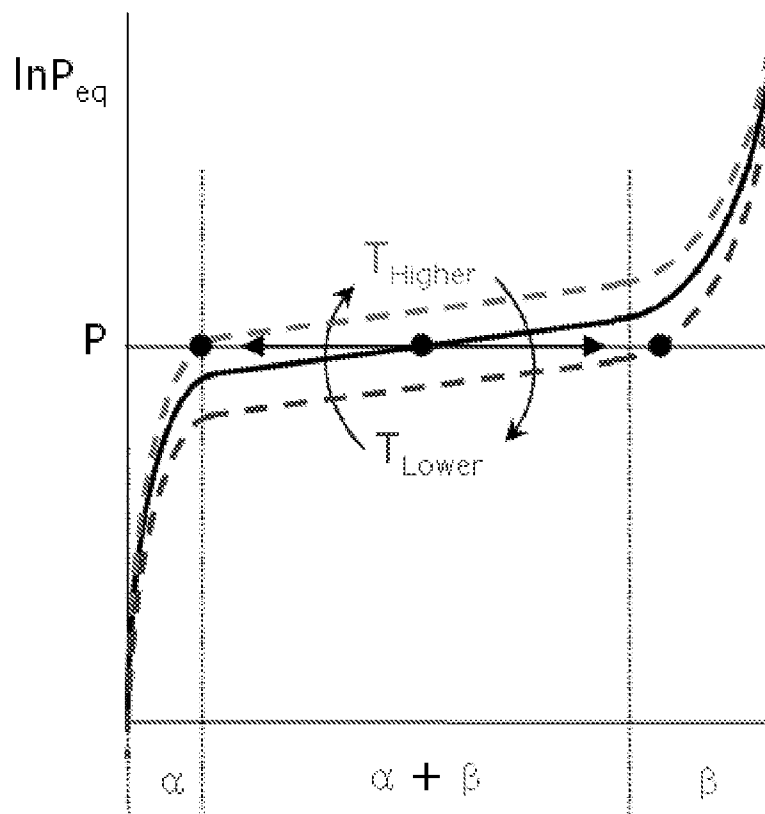


[Fig.2] Pressure concentration Isotherm

The above mentioned hydrogenation process of metallic material is happened not only in lattice structure but also in defects including dislocation structure with multiple atoms and higher bonding energy. This multiple atom formation into the defect is referred to be the cluster. Once the cluster is formed the normal desorption procedure when the hydrogen and/or its isotopes atom transfers out of lattice same atoms in the defects keep clusters because of its higher bonding energy. Therefore where there is more traffic of hydrogen and/or its isotopes there is increased density of the cluster. The basic principle of the proposed invention is to maximize the probability of the cluster formation using the maximized traffic of hydrogen and/or its isotopes in plateau region with hysteresis where alpha and beta phase is co-existed with increased interstitial stress due frequent phase changes. The interstitial stress in the bulk is the another source of increasing the defect density therefore the proposed invention has two fold benefits as 1) cluster formation and increasing its density, 2) creating more defects where new clusters could be formed.

## **2. Method of swinging temperature under isobaric condition**

*The one way to make increased traffic of hydrogen and/or its isotopes atom inner bulk could be realized by changing the bulk temperature while keeping the gas pressure stable and then the equilibrium plateau pressure changes as shown in Fig.3 the pressure concentration isotherms. As plateau changes with the given gas pressure hydrogen and/or its isotopes atom and metal phase is drastically changed for example when the bulk temperature becomes higher the population of beta phase is drastically reduced but the alpha phase is increased and vice versa when the bulk temperature becomes lower. Due to the structural and density discrepancy of both phases the interstitial stress within the bulk is accumulated and it causes to add even more defects where hydrogen and/or its isotopes atoms are trapped while they transfers between both phases.*

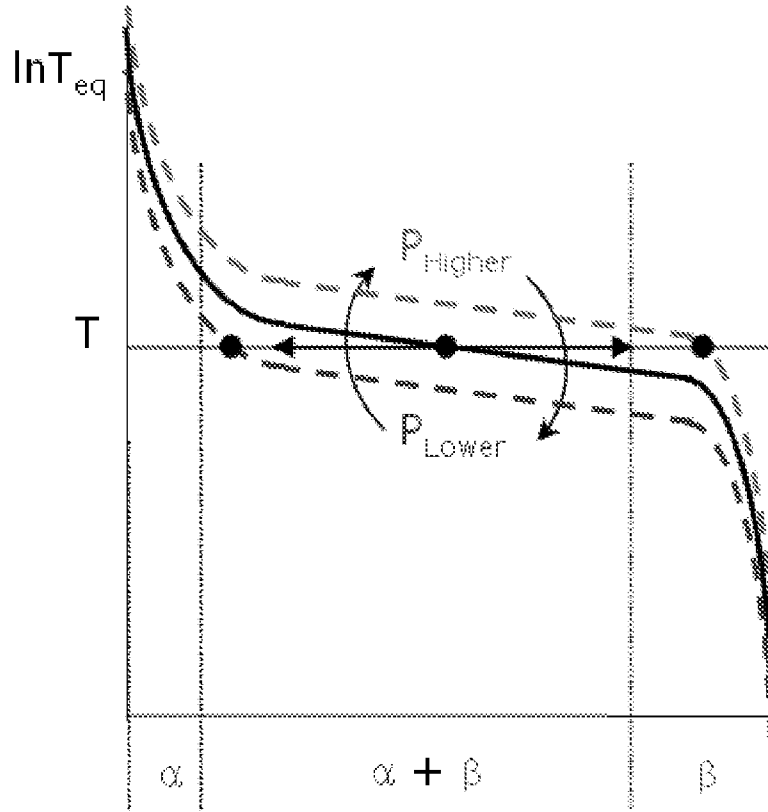


[Fig.3] Pressure Concentration Isotherms

### 3. Method of swinging pressure under isothermic condition

The other method to generate same effect to above mentioned method is to change the gas pressure while keeping the bulk temperature stable and then the equilibrium plateau temperature changes as shown in Fig.4 the temperature concentration isobars. As plateau changes with the given bulk temperature hydrogen and/or its isotopes atom and metal phase is drastically changed. For example when the gas pressure becomes higher the population of alpha phase is drastically reduced but the beta phase is increased and vice versa when the gas pressure becomes lower. Due to the structural and density discrepancy of both phases the interstitial stress within the bulk is accumulated and it causes to add

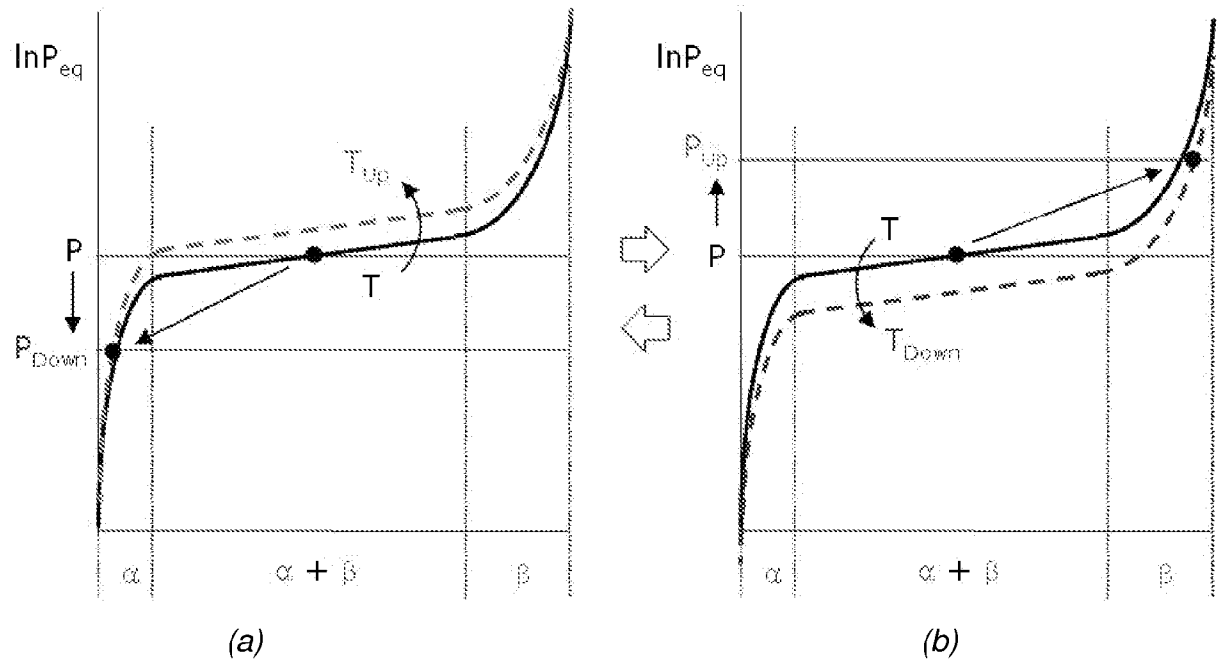
even more defects where hydrogen and/or its isotopes atoms are trapped while they transfers between both phases.



[Fig.4] Temperature Concentration Isobars

#### **4. Combined method of swinging both gas pressure and bulk temperature to control the phase**

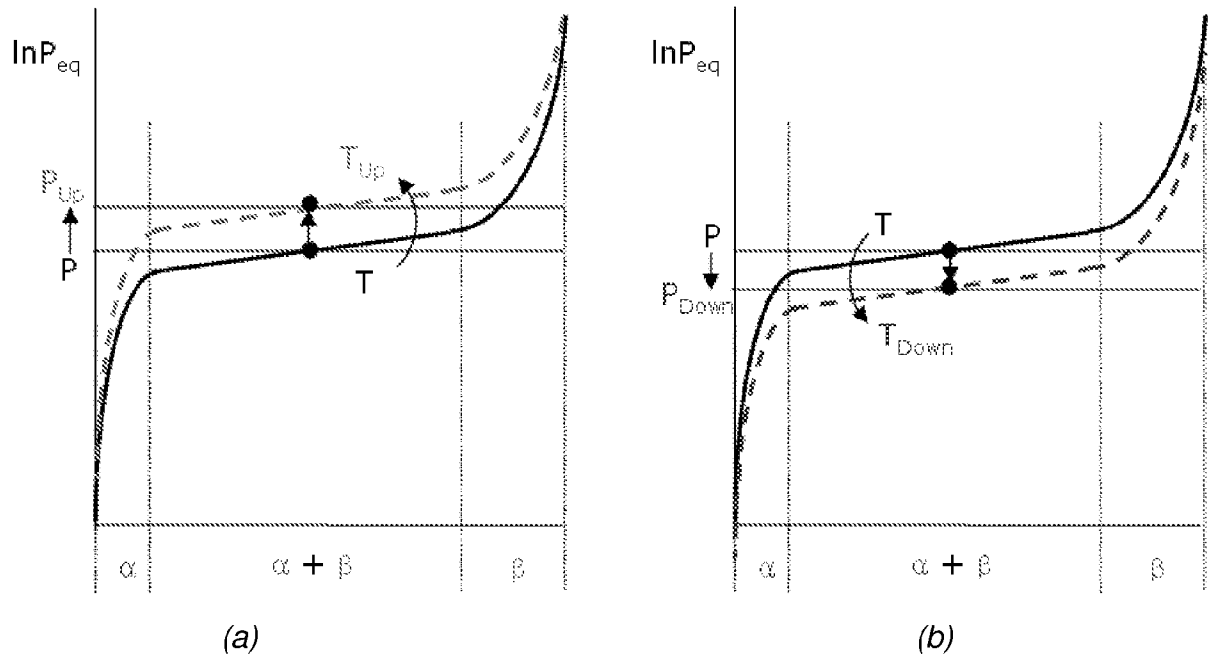
The above described both method could be combined to control bulk phase by use of both gas pressure and bulk temperature swinging as shown in Fig.5. In case when the both of alpha and beta phases are evenly composed in a single bulk by increasing the bulk temperature and simultaneously decrease the gas pressure whole bulk phase is radically turned into the alpha phase as indicated in Fig.5 (a) and vice versa as shown in Fig.5 (b).



[Fig.5] Pressure Concentration Isotherms; (a) Alpha phase formation by temp up and pressure down, (b) beta phase formation by temp down and pressure up

On the contrary when the both bulk temperature and the gas pressure is increased simultaneously there is not drastic changes of the balance in the both phases as shown in Fig.6. If this behavior of phase transition related to the gas pressure and the bulk temperature is properly used in their combination the speed of phase transfer between both phases possibly is controlled and therefore the rate of the cluster formation is controlled as well.





[Fig.6] Pressure Concentration Isotherms; (a) temp up and pressure up; (b) temp down and pressure down.

#### REFERENCES:

US 8603405 B2, Power Units Based On Dislocation Site Techniques.

US 8227020 B1, Dislocation Site Formation Techniques