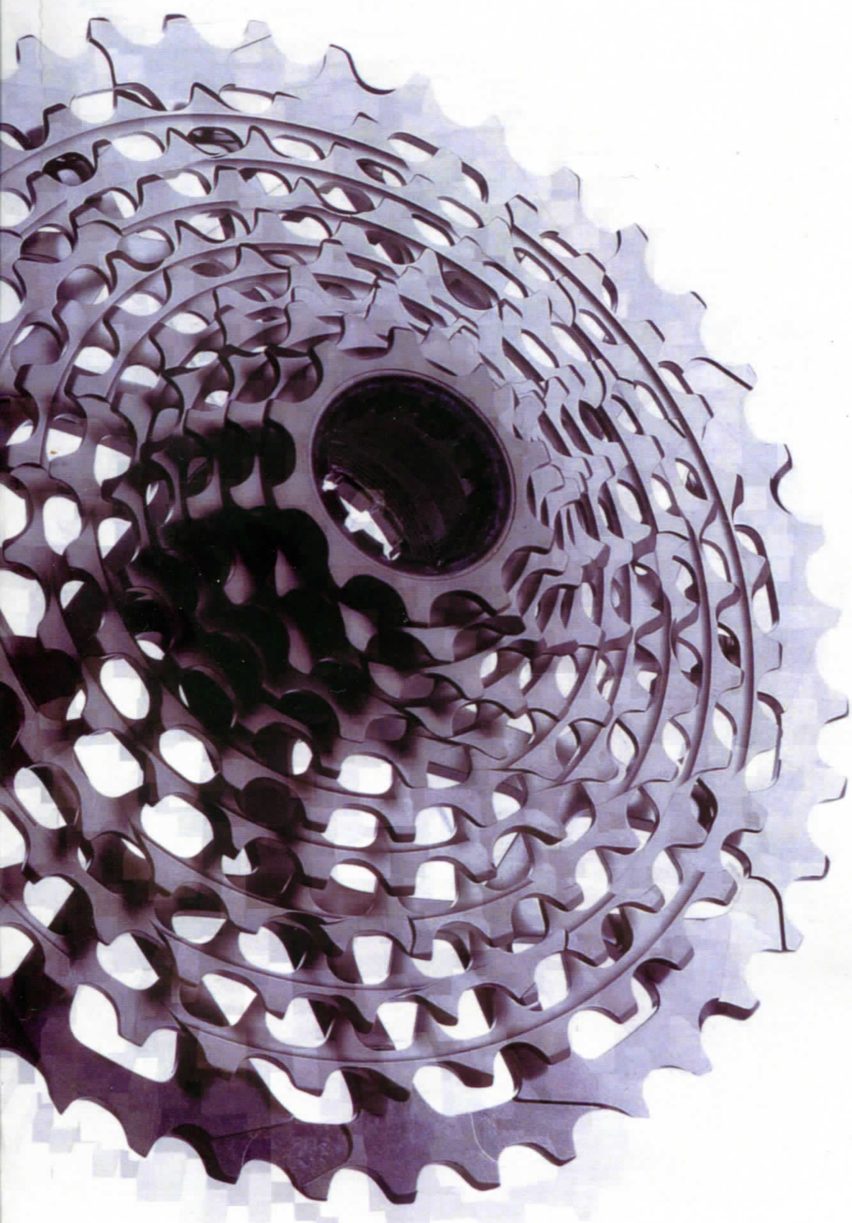
3rd International Symposium on Materials for Energy Storage and Conversion

September 10th-12th, 2018. Belgrade, Serbia

Programme & the Book of Abstracts



VINČA INSTITUTE of NUCLEAR SCIENCES, UNIVERSITY of BELGRADE
HYDROGEN STORAGE INITIATIVE SERBIA

PROGRAMME AND THE BOOK OF ABSTRACTS

3rd International Symposium on Materials for Energy Storage and Conversion - mESC-IS 2018

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POSTER SESSION Monday, 10.09.2018. 17:30-19:30h

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Hydrogen generation in mechanochemical reactor

Milan Petrov[1], Dragan Radulović[1], Ljubiša Andrić[1] and Marina Blagojev[1]
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Hydrogen is considered to be be the fuel of the future. Fuel cells allow that the change of Gibbs function can provide maximum electrical work. Activation with mechanochemical treatment of mineral matter represents a technology that enables us to get fuel with high heat of combustion. The hydrogen generator represents a mechanochemical reactor or a mill with balls in whose operating cylinder is the metal creator in view of grinding bodies, water and abrasive.

Metastable structures

The process of amorphization or the formation of an intermetallic compound can be most easily explained by a hypothetical diagram, as shown in Figure 1.]

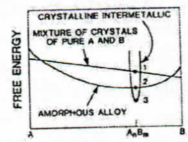

Figure 1. Process of amorphization or the creation of a metastable structure

Active state and excess of free energy

$\Delta G = G^{*} - G$ (1)

G^{*}- Gibbs free energy in activated material

G- Gibbs free energy in non activated material

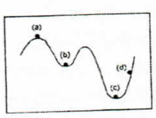

Figure 2. In a stable equilibrium Gibbs free energy is in the lowest possible state (c)

Solid-state processing methods

In the laboratory mill with balls, the hydrogen production was carried out. The volume of the mill was 12 dm³. The mill was placed on horizontal rollers and turned at 60 rpm. The mass of the ball was 10 kg. The mill was closed with a lid with an opening of a circular shape size 1 cm², located on the rubber sleeve. A rubber sleeve with an opening served to accommodate elastic membrane that prevented the exchange of the gas phase between the inner and outer parts of the mill. Quartz sand and water were put in the mill.

Standard molar Gibbs reaction functions

$\Delta_r G^{\ominus} = -RT \ln K$ (2)

By substituting $\Delta_r G^{\ominus}$ in the equation 2 with ΔG from the equation 1, the expression in the form shown in the equation 3 is obtained:

$\ln K = \frac{-\Delta G}{RT}$ (3)

This transformation enables the mechanochemical treatment in the mill (reactor) with steel balls to be presented as a process:

$3Fe + 4H_2O = Fe_3O_4 + 4H_2 \cdots \Delta G = -65{,}2\ kJmol^{-1}$ (4)

Gibbs function of the MH treatment reaction

During MH treatment there was a change in Gibbs free energy and a distortion of the equilibrium of the indicated reaction. After two hours of grinding there is a change in the elastic membrane. It is noted that the elastic membrane (balloon) is filled with gas, which according to the equation 4 is the reaction of hydrogen formation (shown in Figure 3).

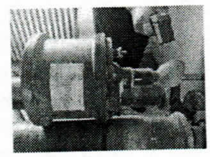

Figure 3. Mehanochemical reaction of hydrogen formation in the mill (reactor)

Change of G at this transition is:

$$\Delta_{pr}G(0{,}65Mbar) = \Delta_{pr}G(1bar) + \left(1 * 10^{-6}\frac{m^3}{mol} * (0{,}65 * 10^{11}Pa - 1 * 10^5 Pa)\right) = \Delta_{pr}G(1bar) + 65\frac{\mathrm{kJ}}{mol}$$

The equilibrium constant is determined according to the general definition for the balanced partial pressure of gases, and for the equation 4 it is shown in the form of the equation 5:

$$K_p = \left\{\frac{p(H_2)}{1}\right\}_{eq} \quad (5)$$

As can be seen from the equation 5, the equilibrium constant has a dimension of pressure (for example, the unit bar).

So for the experimental conditions in the reactor T = 303,15 K, the value of RT is:

$RT = 8{,}315\ JK^{-1}mol^{-1} \cdot 303{,}15\ K = 2520{,}69\ Jmol^{-1}$

Equilibrium constant A has the following value:

$$\ln K = \frac{-(G^{\cdot} - G)}{RT} = \frac{-(65{,}0\ kJmol^{-1} - 65{,}2kJmol^{-1})}{2{,}52069kJmol^{-1}} = 0{,}0793$$

$K = 1{,}083\ bar$

Conclusion

It is interesting to notice the fact that we calculated the work of the mill (reactor) in the dimension $A(=)\ Jmol^{-1}$. It is also important the fact that one of the balls in a mill (reactor) mass m = 6.5 g, in the process of MH treatment, with its operation on the mineral grain size d = 100 µm creates the pressure of 0.65 MPa.

The presented results are a part of research within the Project TR34006, funded by the MEST of the R. Serbia

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Milan Petrov has been employed in ITNMS since 1985. He deals with research in the field of mineral raw materials processing, and especially grinding in these processes. Within the research work he devoted a great deal of attention to the study of energy phenomena in the process of mechanochemical treatment of mineral resources. He is the principal investigator of the project "Mechanochemical treatment of low quality mineral raw materials " funded by the Ministry of Education and Technology Development.

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