

# HYDROGEN CONCENTRATION DEPENDENCE OF PALLADIUM CANTILEVER DEFLECTION IN THE $\alpha$ -PHASE OF THE Pd-H SYSTEM

O.M. Liubymenko

“Donetsk National Technical University”,

Drohobych, Lviv region, Ukraine

E-mail: e.n.lyubimenko@gmail.com

The concentration dependence of the mechanical response of a palladium cantilever during hydrogen absorption within the  $\alpha$ -phase of the Pd-H system was studied. The relationship between the atomic hydrogen concentration (H/Pd), hydrogen pressure, maximum cantilever bending, and the time to reach this maximum was analyzed. The nonlinear nature of the dependence of the bending on the hydrogen concentration was established. In the low concentration zone (up to  $\sim 0.02$  H/Pd), a decrease in bending is observed, which is explained by the stabilizing effect of hydrogen atoms in the interstitial spaces of the palladium lattice. In the range of  $0.03 \dots 0.04$  H/Pd, the dependence becomes almost linear due to the expansion of the  $\alpha$ -PdHx lattice. A further increase in the hydrogen concentration is accompanied by an increase in the cantilever bending. The results obtained are important for the creation of micromechanical hydrogen sensors.

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In recent years, special attention has been paid to the study of micromechanical effects that arise during the absorption of hydrogen by metals. One of the promising methods for studying such processes is the use of microcantilevers, which have a high sensitivity to the internal stress that arises in the material when its chemical composition changes. When palladium is saturated with hydrogen, the interatomic distances change, which leads to the expansion of the crystal lattice and the emergence of internal concentration stresses. These processes manifest themselves in the form of a cantilever bend, which can be recorded with high accuracy.

The study of the dependence of the deflection of a palladium cantilever on the hydrogen concentration allows us to obtain important information about the mechanisms of interaction of hydrogen with the crystal lattice of palladium, as well as about the kinetics of the diffusion and distribution of hydrogen in the material. Of particular interest is the region of the  $\alpha$ -phase of the Pd-H system, in which hydrogen dissolves in the interstitial spaces of the palladium crystal lattice, forming a solid solution.

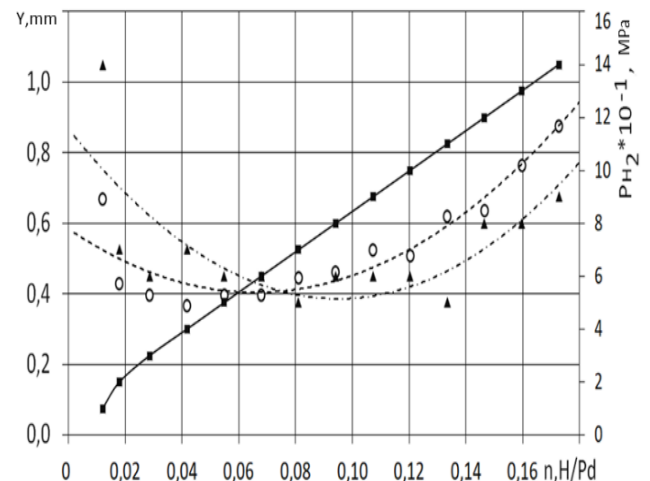
The aim of this work is to study the dependence of the maximum deflection of a palladium cantilever on the atomic concentration of hydrogen in the  $\alpha$ -phase of the Pd-H system, as well as to analyze the time to reach the maximum deflection at different hydrogen concentrations.

The experimental study was carried out using a palladium cantilever placed in a vacuum chamber, into which hydrogen was metered. During the experiment, changes in the cantilever deflection were recorded at different hydrogen pressure values.

The change in concentration was achieved by successive hydrogen inlets into the chamber. At each inlet, the maximum deflection of the cantilever and the time required to reach this maximum were recorded.

The cantilever deflection was recorded using an optical measurement system that provides high accuracy in determining micromechanical deformations. The obtained experimental data (Figure) allowed us to construct the dependences of the maximum cantilever

deflection, hydrogen pressure, and the time to reach the maximum deflection on the hydrogen concentration in palladium.



Dependence of the maximum bending of a palladium cantilever and hydrogen pressure on the atomic hydrogen concentration H/Pd

The analysis of experimental dependences was carried out using mathematical approximation methods. To describe the dependence of the maximum deviation of the cantilever on the hydrogen concentration, a polynomial function was used:

$$Y_{\max} = 2 \cdot 10^6 n^6 - 1 \cdot 10^{6n^5} + 327569 n^4 - 40076 n^3 + 2580.6 n^2 - 80.435 n + 1.2992 \text{ mm} \quad (R^2 = 0.9701), \quad (1)$$

$n$  is the concentration of atomic water, H/Pd.

The time to reach the maximum is the greatest in the low concentration zone, namely in the region of ideal and pseudo-ideal solid solutions up to  $\sim 0.02$  H/Pd, then - fluctuates. Mathematically, it can be described by the polynomial

$$t_{\max} = 167214 n^4 - 66875 n^3 + 9612.7 n^2 - 571.36 n + 17.3, \text{ s} \quad (2) \quad R^2 = 0.6862.$$

The high value of the coefficient of determination indicates a good correspondence of the model to the experimental results.

The analysis of the experimental data showed that the dependence of the maximum cantilever deflection on the hydrogen concentration has a complex nonlinear character. In the region of low hydrogen concentrations, a significant change in the bending magnitude is observed, associated with the peculiarities of hydrogen dissolution in the palladium crystal lattice.

At hydrogen concentrations of approximately 0.02 H/Pd, the system corresponds to the region of ideal and pseudo-ideal solid solutions. In this region, a sharp decrease in the maximum cantilever deflection is observed. This behavior can be explained by the stabilizing effect of hydrogen atoms introduced into the interstitial spaces of the palladium crystal lattice. The introduction of hydrogen leads to a redistribution of internal stresses arising in the material, which affects the nature of the mechanical deformation of the cantilever.

With a further increase in the hydrogen concentration, a change in the nature of the dependence is observed. In the concentration range of 0.03...0.04 H/Pd, the dependence of the cantilever deflection on the concentration becomes almost linear. This behavior is associated with the process of hydrogen dissolution in the interstitial spaces of the  $\alpha$ -PdH<sub>x</sub> crystal lattice. The introduction of hydrogen atoms leads to an increase in the lattice parameter and its uniform expansion.

In the concentration range of 0.03...0.06 H/Pd, a region is observed where the dependence of the cantilever deflection is characterized by the presence of a plateau. In this region, the system cannot be considered as an ideal solid solution. The interaction between hydrogen atoms leads to a change in the distribution of internal stress in the crystal lattice.

With a further increase in the hydrogen concentration to values of 0.07 H/Pd, a gradual increase in the maximum cantilever deflection is observed. This effect is associated with the strengthening of interatomic repulsive forces between hydrogen atoms located in the interstitial spaces of the crystal lattice. As a result, the palladium lattice expands further and the mechanical deformation of the cantilever increases.

At hydrogen concentrations above 0.07 H/Pd, a further increase in the deflection is observed. This behavior is consistent with known data on the dilation of the palladium crystal lattice when hydrogen is dissolved.

Of particular interest is the analysis of the time to reach the maximum deflection of the cantilever. Experimental data show that at low hydrogen concentrations the time to reach the maximum deflection is the longest. This is because in this area the process of hydrogen saturation of palladium with hydrogen is determined mainly by the diffusion transfer of hydrogen into the surface layers of the metal.

A small gradient of hydrogen concentration leads to a relatively slow penetration of hydrogen into the depth of the material. In addition, hydrogen adsorption on the palladium surface plays a significant role.

With increasing hydrogen concentration, the time to reach the maximum deflection decreases and then stabilizes. This indicates that the processes of hydrogen

transport to the surface, its diffusion into the volume of the material and the accumulation of internal stresses begin to occur simultaneously.

Additional confirmation of this is the residual deformations of the cantilever observed at high hydrogen concentrations. At hydrogen concentrations greater than 0.09 H/Pd, after the experiment, residual changes in the shape of the cantilever remain, the magnitude of which increases with subsequent hydrogen introduction. In this case, the magnitude of the residual deformations corresponds to the region of elastic deformations of the material.

The results obtained indicate the complex nature of the interaction of hydrogen with the crystal lattice of palladium. The mechanical response of the cantilever is determined by a combination of several processes, including hydrogen adsorption on the surface, its diffusion into the volume of the metal, redistribution of internal stresses and changes in the parameters of the crystal lattice.

## CONCLUSIONS

1. An experimental study of the dependence of the deflection of a palladium cantilever on the hydrogen concentration in the  $\alpha$ -phase of the Pd-H system at a temperature of 350 °C was conducted.

2. It was established that the dependence of the maximum deflection of the cantilever on the hydrogen concentration has a complex nonlinear character.

3. In the region of low hydrogen concentrations (up to 0.02 H/Pd), a decrease in the maximum deflection is observed, associated with the stabilizing effect of hydrogen atoms in the palladium crystal lattice.

4. In the concentration range of 0.03...0.04 H/Pd, the dependence of the cantilever deflection becomes close to linear due to the uniform expansion of the  $\alpha$ -PdH<sub>x</sub> crystal lattice.

5. With increasing hydrogen concentration, an increase in the maximum deflection is observed, due to the strengthening of interatomic interactions and lattice dilation.

6. It is shown that the time to reach the maximum deviation is the largest at low hydrogen concentrations and decreases with increasing hydrogen content in palladium.

7. The results obtained can be used to develop highly sensitive hydrogen sensors and a deeper understanding of the mechanisms of hydrogen interaction with metals.

## REFERENCES

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## ЗАЛЕЖНІСТЬ ВИГИНУ ПАЛАДІЄВОГО КАНТИЛЕВЕРА ВІД КОНЦЕНТРАЦІЇ ВОДНЮ В $\alpha$ -ФАЗІ СИСТЕМИ Pd-H

*О.М. Любименко*

Досліджено концентраційну залежність механічного відгуку паладієвого кантилевера під час поглинання водню в межах  $\alpha$ -фази системи Pd-H. Проаналізовано взаємозв'язок між атомною концентрацією водню (H/Pd), тиском водню, максимальним вигином кантилевера та часом досягнення цього максимуму. Встановлено нелінійний характер залежності вигину від концентрації водню. У зоні низьких концентрацій (до  $\sim 0,02$  H/Pd) спостерігається зменшення вигину, що пояснюється стабілізуювальною дією атомів водню в міжвузлях ґратки паладію. У діапазоні  $0,03 \dots 0,04$  H/Pd залежність стає майже лінійною через розширення ґратки  $\alpha$ -PdH<sub>x</sub>. Подальше зростання концентрації водню супроводжується збільшенням вигину кантилевера. Отримані результати важливі для створення мікромеханічних сенсорів водню.