#### INTERACTION OF THE ELECTROMAGNETIC RADIATION WITH THE SURFACE OF PALLADIUM HYDRIDE CATHODES

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The change of the electronic density of metallic Pd due to the hydride formation and to the build-up of the double layer, rising at the metal-dielectric interface when an electric field is applied, is involved in the variation of the metal dielectric function. A model including also metal surface roughness has been developed to take into account such modifications.

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## Introduction

The dissolution of hydrogen within a metal lattice and the formation of a metal hydride greatly perturb the electrons and phonons of the host material. Several are the relevant observed effects

- The generally observed expansion of the lattice, often including a change in the crystal structure, involves a modification of the symmetry of the states and a reduction of the band width.
- The attractive potential of the protons affects those metal wavefunctions which have a finite density at the H site and leads to the so called metal hydrogen bonding band below the metal dband.
- The additional electron brought by the H atoms into the unit cell produces a shift of the Fermi level.

Consequently, the electronic Density of State of Palladium changes as deuterium solubilized inside metal lattice increase.



Fig. 1 - Total Density of States at the Fermi level plotted versus hydrogen concentration in PdHx

## Model of the Electrochemical Interface

The electrochemical interface is well represented by a double layer structure in contact with a space of charges



$$\frac{d\varphi}{dx} = -\left(\frac{8KTn_0}{\varepsilon_0}\right)^{1/2} \sinh\left(\frac{ze\varphi}{KT}\right)$$

$$\varphi = \frac{2KT}{ze} \ln\left(\frac{1 + \beta e^{-\tilde{k}x}}{1 - \beta e^{-\tilde{k}x}}\right)$$

$$\varphi_2 = \varphi_0 + \left(\frac{d\varphi}{dx}\right)_{x=x_2} x_2$$

$$\sigma^{m} = \left(8KT\varepsilon_{0}n_{0}\right)^{\frac{1}{2}} \sinh\left(\frac{ze\varphi_{2}}{2KT}\right)$$

$$\widetilde{k} = \left(\frac{2n_0 z^2 e^2}{\varepsilon_0 kT}\right)^{\frac{1}{2}}$$

$$\beta = \tanh(ze\varphi_0 4KT)$$

$$E_{dl} = \frac{d\varphi}{dx}\Big|_{x_2}$$

$$\rho_0 = 250mV$$
  
 $E_{dl} = 10^{8}V/m$ 

## **PdH Dielectric Function Estimation**

The purpose is to obtain a reasonable, consistent dielectric function value suitable to be used in our model



Fig.2- Dielectric function real component, palladium hydride

Fig. 3- Dielectric function imaginary component, palladium hydride

Double layer is characterized by a high density of charges: it is necessary to describe a metal foil having on its surface a very high charge density, which results in an intense electrostatic field

### • The dielectric function variation related to surface charge density is



The shift to negative values due to surface charge is shown

versus angular frequency. The shift to higher values due to surface charge is shown<sup>7</sup>

## **Surface Plasmons**

> Surface plasmons (polaritons) are quanta of plasma oscillations created by the collective oscillation of electrons on a solid surface.

Surface plasmons may be generated by mechanisms able to produce charge separation\_between Fermi level electrons and a background of positive charges (i.e. lattice atoms)



Surface Plasmons Wave Vector x component dispersion relation is expressed by

$$K_{x} = \frac{\omega}{c} \sqrt{\frac{\varepsilon_{d} \hat{\varepsilon}}{\varepsilon_{d} + \hat{\varepsilon}}}$$

> Under certain conditions one could use the simplified expression:

$$K_{x}' = \frac{\omega}{c} \sqrt{\frac{\varepsilon_{d}(\omega^{2} - \omega_{p}^{2})}{\omega^{2}(\varepsilon_{d} + 1) - \omega_{p}^{2}}}$$

$$\omega_p^2 = \frac{Ne^2}{m_{eff}\varepsilon_0}$$

## **Surface Plasmons Excitation Conditions**

### - Prism Coupling





Fig.6 - Matching condition given by interception between s.p. and laser beam dispersion law, achievable using a prism coupler - Roughness Coupling

$$K_x = \frac{\omega}{c}\sin\theta \pm \Delta K_x = K_{sp}$$



Fig.7 - Matching condition given by laser beam wave vector increment due to a corrugation lattice

# Electro-Magnetic field Enhancement due to Surface Plasmons Excitation

Surface Plasmons resonance could give rise to a huge local field enhancement, due to a focusing effect: a broad e.m. wave is confined in a surface.

This phenomenon could be understood considering the wave vector component perpendicular to the interface between the two media:

$$K_{z^2} = \frac{\omega}{c} \sqrt{\frac{\hat{\varepsilon}^2}{\hat{\varepsilon} + \varepsilon_1}}$$

$$K_{z1} = \frac{\omega}{c} \frac{\varepsilon_1}{\sqrt{\hat{\varepsilon} + \varepsilon_1}}$$

The field enhancement could be in a phenomenological way expressed as

$$\frac{\left|\vec{E}_{j}\right|^{2}}{\left|\vec{E}_{0}\right|^{2}} \approx \frac{\left|K_{zj}^{\prime\prime}\right|}{K_{x}^{\prime\prime}}$$

Enhancement of about 10<sup>2</sup> factor could be obtained in this classical calculation. On appropriate structures and by quantum mechanical computation the enhancement factor could be equal to several magnitude orders



Fig.8 - Electromagnetic Field due to SP excitation, arbitrary units

## **Palladium Cathodes Roughness**



L72a(207-225)RA\_4.jpg



### L68(0-20)RAE\_5.jpg





### L51(43-81)RAE\_5.jpg

### L68(20-40)RAE\_3.jpg





L55(215-254)RAE\_7.jpg

L56(6-26)RAE\_5.jpg

Sample	Roughness (µm)	Surface Profile Average Wave Length (µm)
L72a(207-225)RA	0.024	2
L68(0-20)	0.109	2.3
L68(20-40)	0.175	3
L51(43-81)RAE	0.112	1.8
L55(215-254)RAE	0.132	1.6
L56(6-26)RAE	0.205	1.5

### **Rough Surface Reflectance Simulation**

A surface Plasmon can not be excited by direct impinging of an electromagnetic radiation on a smooth surface

Deepenings

- A rough surface increases incoming electromagnetic wave momentum
- Modelling: Laser Angular Reflectance from gratings





S10 O3









## **Finite Element Method Model**

- Previous Model:
  - > No information on Electromagnetic Field localization
  - Source terms can not be included in the Analytical Model
- FEM implemented to solve differential Maxwell equations.
- Adequate boundary conditions are needed: Perfectly Matched Boundary Conditions (PML)



in free space



in a two semi-infinite media domain







Fig. 12- Magnetic field originated by a surface current flux





Fig. 13- Electric field distribution originated by an alternate surface current density flowing on a corrugated interface between air and PdHx

## Conclusions

Description of Pd samples surface under cathodic polarization has been performed by including the effects of high charge density at the inter-phase

On suitable surfaces electron plasma oscillation may occur. Their frequency is depending on the material electronic properties and surface profile properties

The models developed show that under adequate conditions strong electromagnetic field localization and magnification arises.

Advanced modelling of process occurring at the interface and into the bulk is the first step towards material engineering