H/H_2 Phases in Ni(111) Nanogaps, Sensing and the Binding Energy

Sveinn Ólafsson, Tryggvi K. Tryggvason, Vilhjálmur Ásgeirsson and Egill Skúlason

Science Institute, University of Iceland, 107 Reykjavik, Iceland

ICCF18 Conference July 21-27 2013 University of Missouri Columbia USA

Sensing the occupancy of H or H_2 atoms in a gap

Making nanogaps in material where gases can adsorb and react with possibility of sensing the event is difficult. Here we present an experimental approach that could achieve this function.

Two films are grown on a flat surface having island type of growth, each film can be characterised by the film roughness accessible by X-ray reflectivity measurements. The films are brought into contact by placing the other on top of the other, as seen in the figure 1b. The contact conductivity and noise can be measured and monitored in time with the sample holder placed in a small UHV chamber.

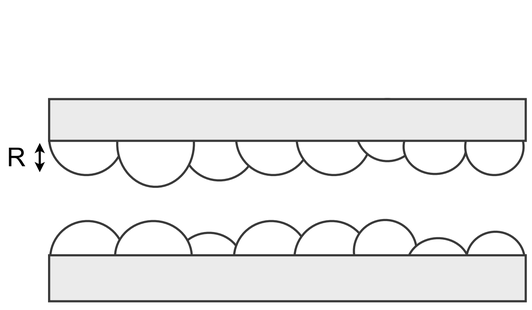

Figure 1a. Two films with roughness Ra and distance h.

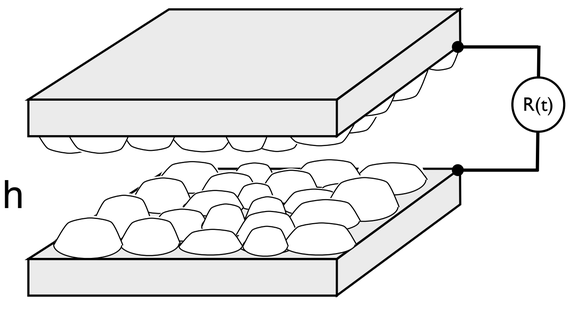

Figure 1b. Conductivity and current noise is monitored.

The distance between the two substrates h can be varied by pressing on the top substrate with a constant force. The statistical variations in the gap distance in such an experimental arrangement can be calculated assuming perfectly ideal flat substrate with films of thickness d and roughness Ra. Results of such simulation are presented in next figures where the island or film thickness d is on average 3 monolayers and roughness variation is 1.23. Histograms of distances is presented for the cases h=8 and h=6 monolayers.

For each case a contour plot is given showing the regions where contact has been made and also regions where distance between atoms on bottom and top substrates is less than 3 monolayers. In these regions adsorbed hydrogen atoms could contribute to conductivity in addition to the conductivity through the contact areas.

A variation of this method would be to use ultra thin nano powder layer pressed between these two films.

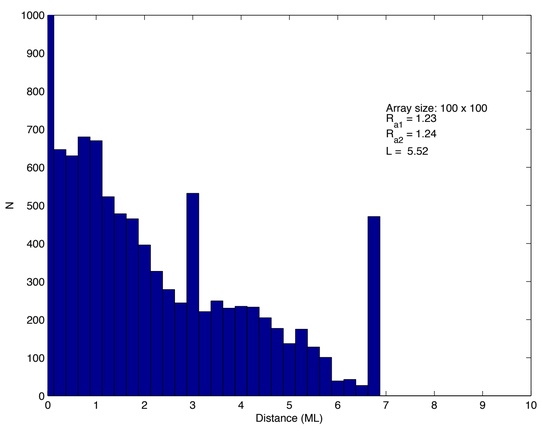

Figure 2a. Histogram of the bottom atom to the top atom distances a. Here is h=8 ML.

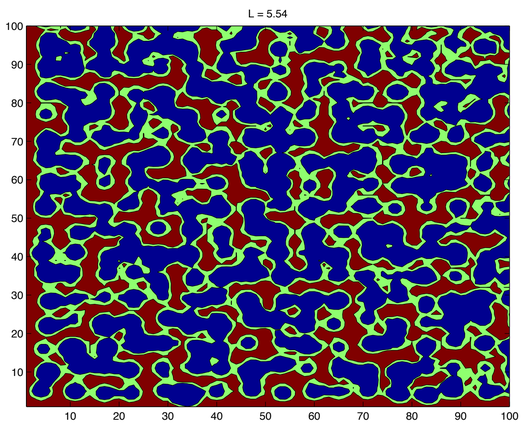

Figure 2b. Color mapping of distances. Blue colored region is where contact has been obtained. Light green is region (a<3 ML) where Hydrogen can give contribution to conductivity.

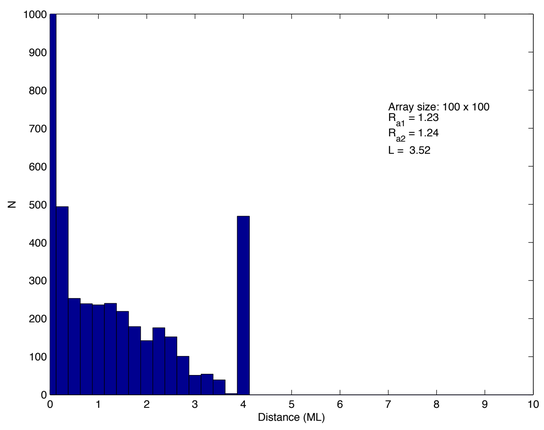

Figure 3a. Histogram of the bottom atom to the top atom distances a. Here is h=6 ML.

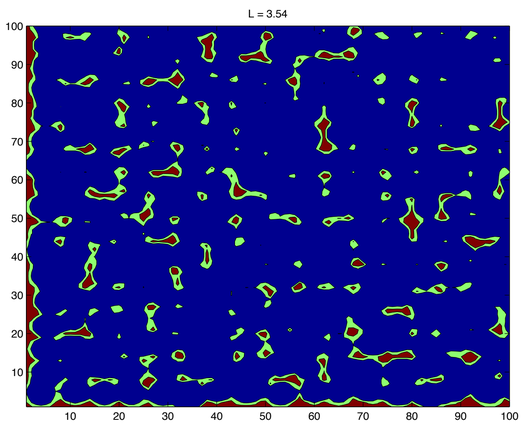

Figure 3b. Color mapping of distances. Blue colored region is where contact has been obtained. Light green is region (a<3 ML) where hydrogen can give contribution to conductivity.

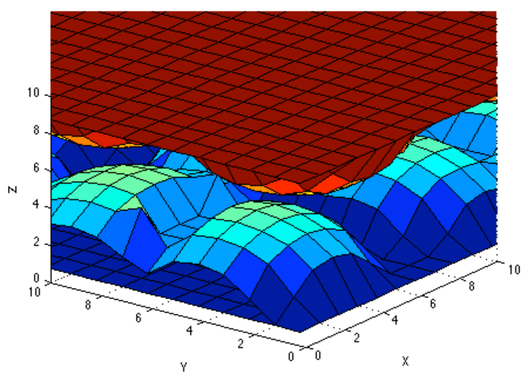

Figure 4. Zoomed view of the two films

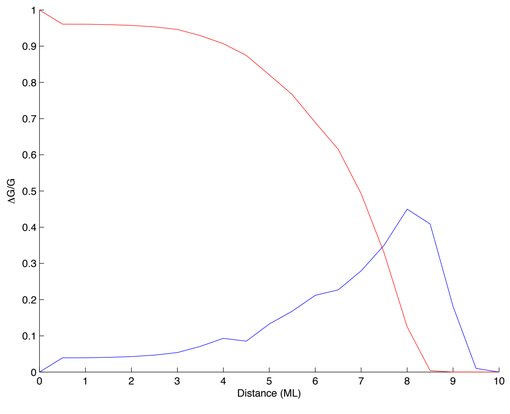

Figure 5. Shows the area of the two regions relative to the whole substrate area as the gap distance is reduced from h=8 ML. Blue line is the hydrogen region, red line is the contact region.

Assuming that the conductivity of hydrogen region is the same as the contact region, the maximum sensitivity in sensing the hydrogen region or possibly LENR related event is found at gap distance of h≈8 monolayers for these two facing samples. [1]

Binding energy of H and H_2 in Ni nanogap

DFT electronic structure calculations were performed on Ni cell consisting of 16 Nickel atoms and one missing Ni layer mimicking a variable Ni gap structure. Binding energy of 8 H atoms chemisorbed on Ni(111) surface was calculated as function of gap distance using nickel 1ML=0.203nm, measured as distance from centre of the facing Ni-atoms. The FCC closed packed structure layering is ABCA-gap-ABCA- giving the simplest unit cell for the calculation. Binding energy of extra 4 H atoms were calculated as well.

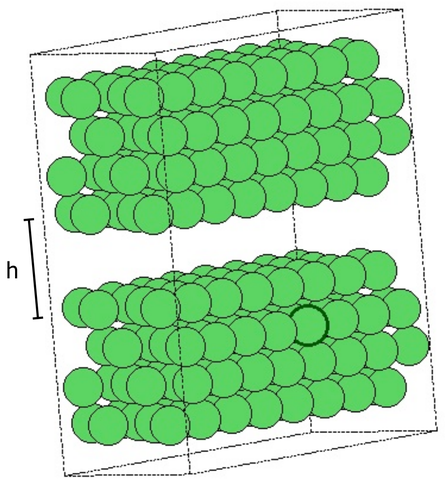

Figure a. Clean Ni gap with one Ni ML removed and gap distance increased

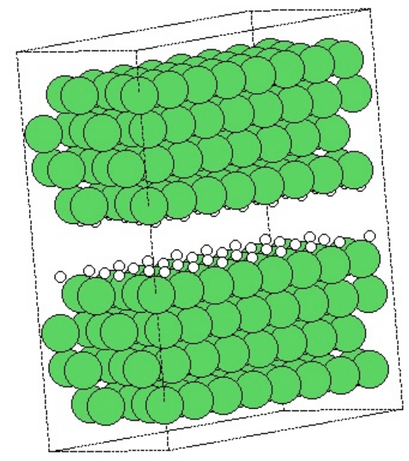

Figure b. Chemisorbed H on Ni(111)

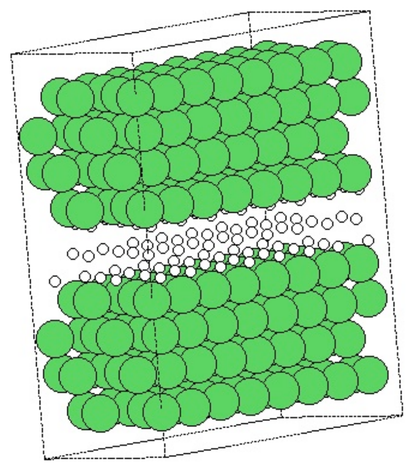

Figure c. Chemisorbed H and H atom layer.

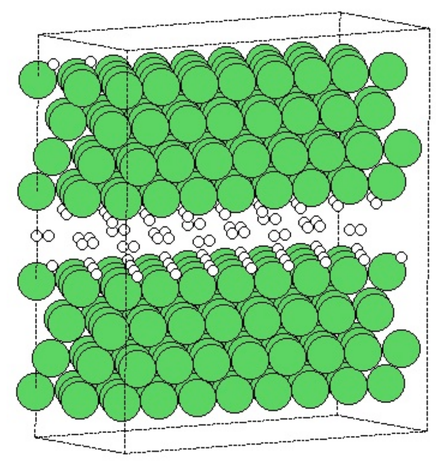

Figure d. Chemisorbed H and H_2-layer

Gap distance h [ML]	ΔE H on Ni (111) surface	ΔE 4 H atoms added
1.5	0.02	0.76 (H-layer)
2.0	-0.31	0.84 (H-layer)
2.5	-0.37	0.85 (H top site)
3.0	-0.37	0.14 (H2 gas)
4.0	-0.37	-0.01 (H2 gas)
5.0	-0.37	-0.02 (H2 gas)

Results are found in tabel A. Binding energy ΔH of H (eV/H-atom) with respect to H_2 gas phase. Negative values lead to binding or absorption depending on temperature and H_2 gas pressure. For comparison β-phase of $PdH_{0.6}$ has binding energy ΔH of -0.2 eV/H-atom.

H and H_2 binding energy calculation conclusions

- Fully Hydrogen chemisorbed Ni(111) surface is stable at gap distances larger than 1.5 ML Nickel with binding energy of -0.37 eV/H-atom.
- When adding H atoms in the gap, (Electrolytical charging, plasma charging, electric field gradient? or closing partially the gap?) there is possibility of formation of H-layer phase at smallest distances.
- At larger distances the H-atomic layer move and settles on top site position of the Ni surface.
- Finally as the gap opens further up the extra H-atoms recombine into H_2 molecules

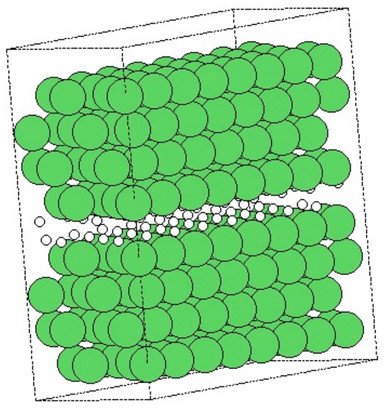

Figure e. Unstable with respect to H_2 gas, chemisorbed H on Nickel (111) gap at small gap distance

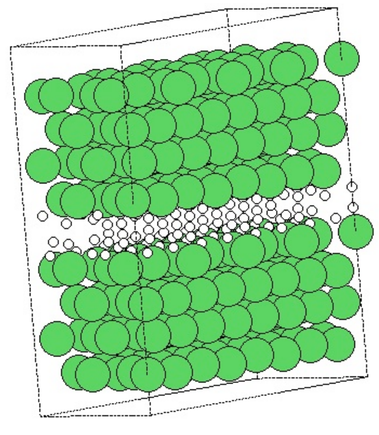

Figure f. More unstable with respect to H_2 gas, chemisorbed H on Nickel (111) gap (top site also) at small gap distance

1. Conduction Mechanism in a Molecular Hydrogen Contact, K. S. Thygesen and K. W. Jacobsen PRL 94, 036807 (2005)

This work is funded by the Icelandic Research Fund, the University of Iceland Research Fund