

# Hydrogenated Amorphous Silicon

Yifan Yuan

1/26/2021

Chapter 1 Introduction to hydrogenated amorphous silicon

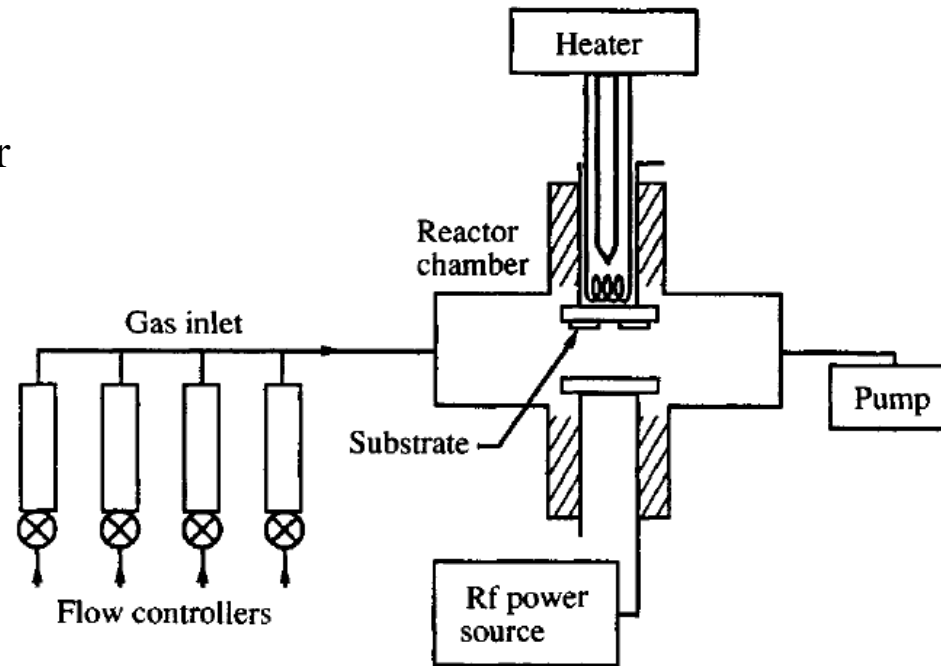
**Chapter 2 Growth and structure of amorphous silicon**

# 1. Growth of a-Si:H

- Plasma decomposition of silane gas,  $\text{SiH}_4$
- Decomposition temperature  $450\text{ }^\circ\text{C}$  for  $\text{SiH}_4$  in the absence of plasma.
- Polycrystalline or epitaxial silicon by high temperature pyrolytic decomposition.
- Amorphous films can be grown by pyrolytic decomposition of  $\text{SiH}_4$  less than  $550\text{ }^\circ\text{C}$ , but low quality due to lack of hydrogen.
- At lower temperatures, **plasma** plays a role to dissociate the silane molecule.

Fig. 2.1. Schematic diagram of a typical rf diode plasma reactor for depositing a-Si:H and alloys.

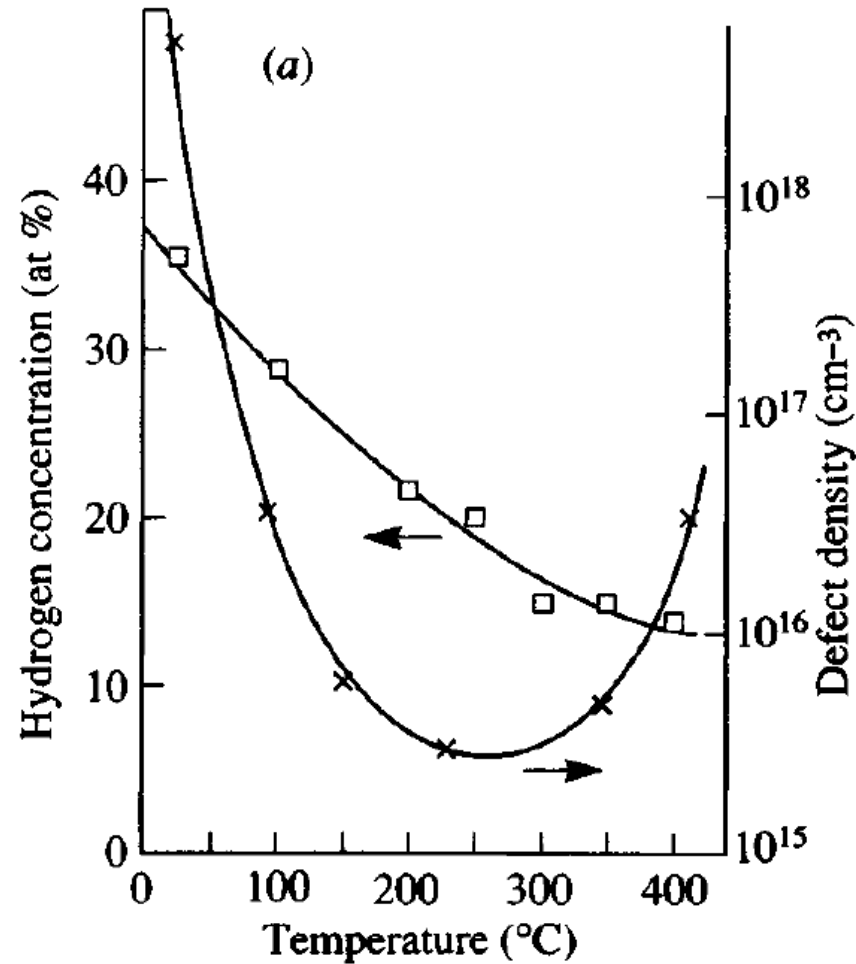
Plasma enhanced chemical vapour deposition (PECVD).



**0.1–1 Torr,**

the optimum pressure to sustain the plasma.

# 1. Growth of a-Si:H

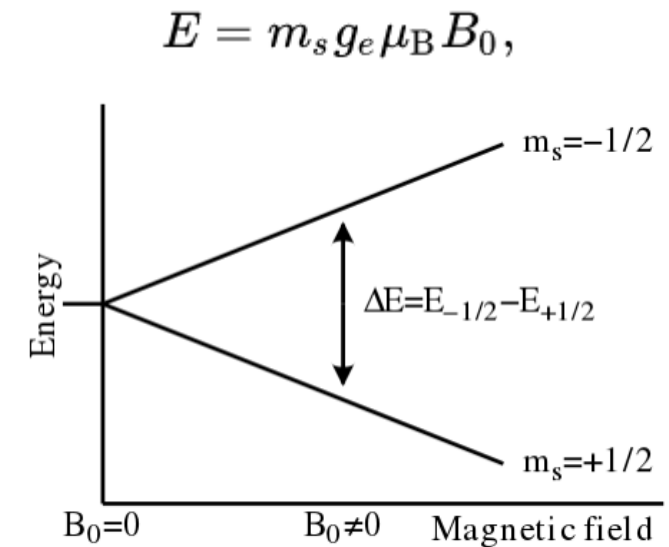
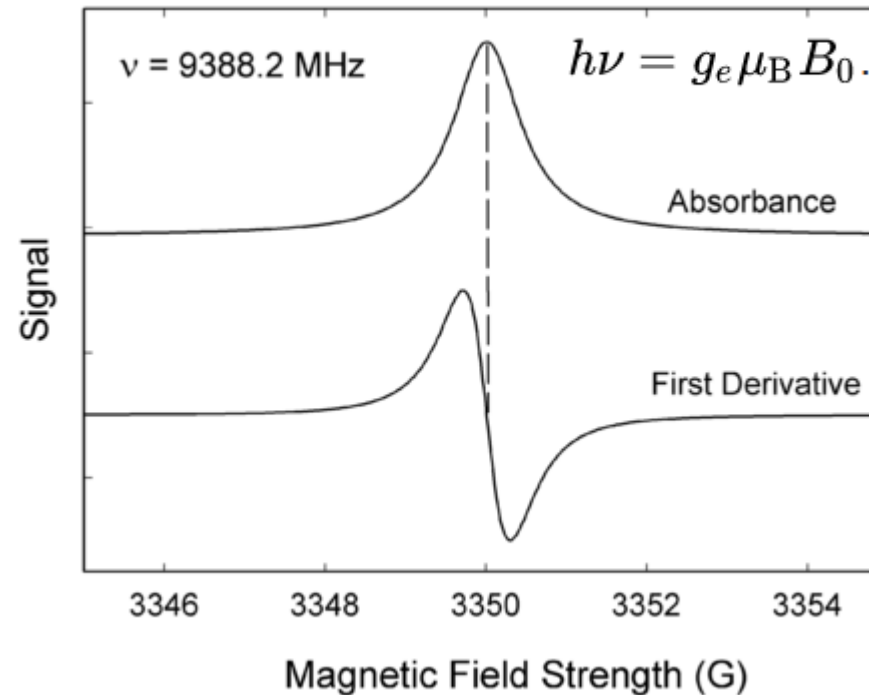


Maxwell-Boltzmann distribution

$$\frac{n_{\text{upper}}}{n_{\text{lower}}} = \exp\left(-\frac{E_{\text{upper}} - E_{\text{lower}}}{kT}\right)$$

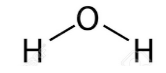
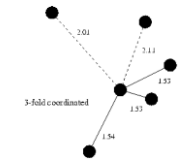
Defects are estimated by photo-induced electron spin resonance (ESR) measurements which provide both quantitative and qualitative information about unpaired spins in a material.

An unpaired electron can change its electron spin by either absorbing or emitting a [photon](#) of energy  $h\nu$  such that the resonance condition,  $h\nu = \Delta E$ , is obeyed.



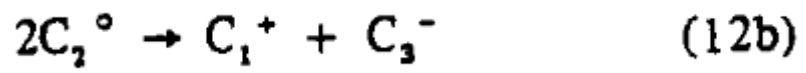
# Bonding defects (D)

three-fold coordinated



The **D-** center was assumed to be a dangling bond and the **D+** center was assumed to be three-fold coordinated atoms

$C_n^o$ : chalcogen element, coordination number (n), neutral (o)



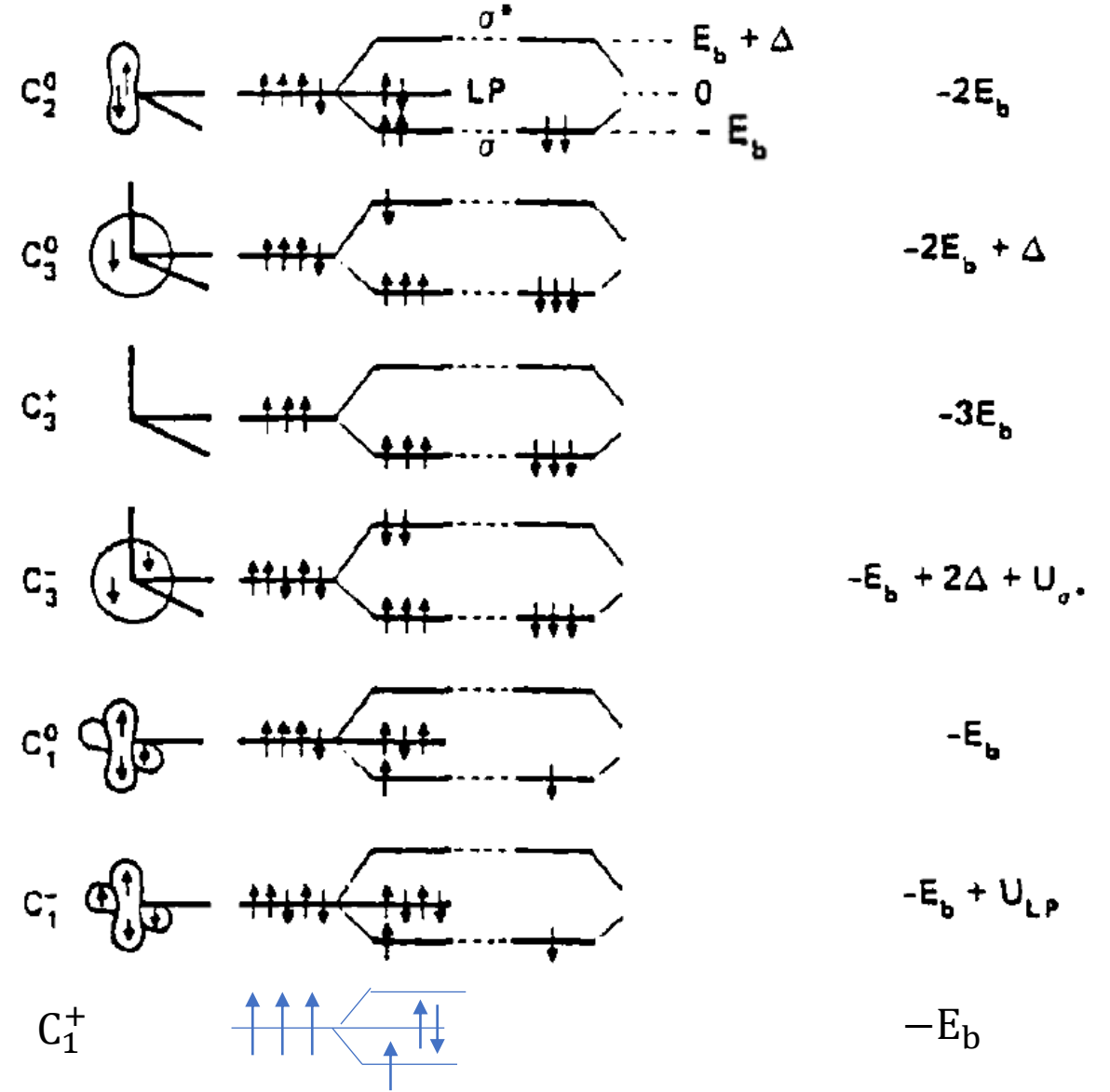
$$-4E_b \rightarrow -E_b + (-E_b + 2\Delta + U_{\sigma*})$$

Defect formation energy:  $E_b + 2\Delta + U_{\sigma*}$

$U_{\sigma*}$  is a correlation energy associated with the electron pair in a non-bonding orbital

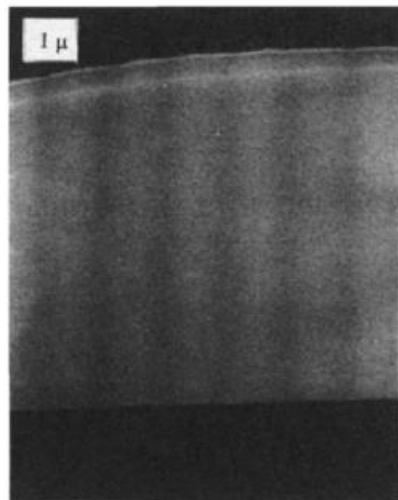
$U_{LP}$  correlation energy associated with two sets of long pairs

CONFIGURATION    p-LEVEL OCCUPATION    ENERGY/CONFIGURATION



## 2. The morphology of film growth

Side view

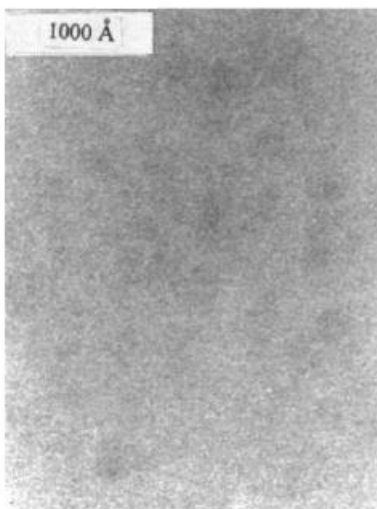


(a)

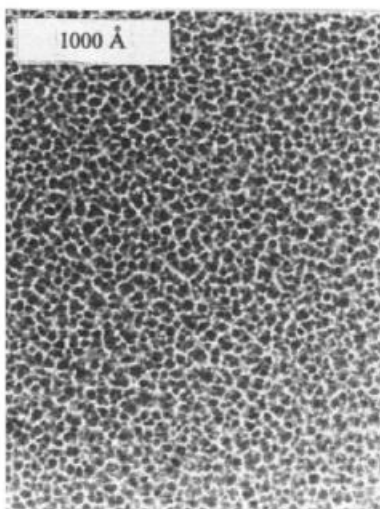


(b)

Top view



(c)



(d)

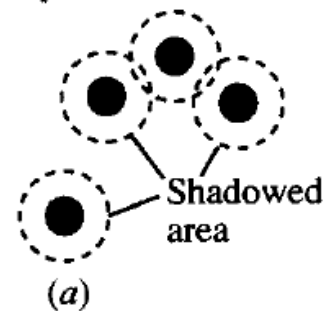
Film in (a)(c) is deposited from pure silane at low rf power

Film in (b)(d) is deposited from silane diluted to 5 % in argon and at high rf power

Dilution with argon causes the films to grow with a columnar morphology in the a-Si: H film

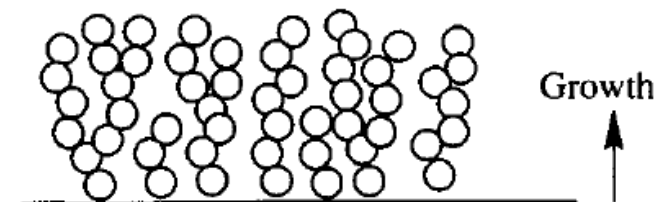
Fig. 2.6. Illustration of (a) the shadowing effect of atoms on the growth surface, and (b) the resulting chain-like growth morphology when the sticking coefficient is high.

Top view



(a)

Side view



(b)

Atomic scale shadowing

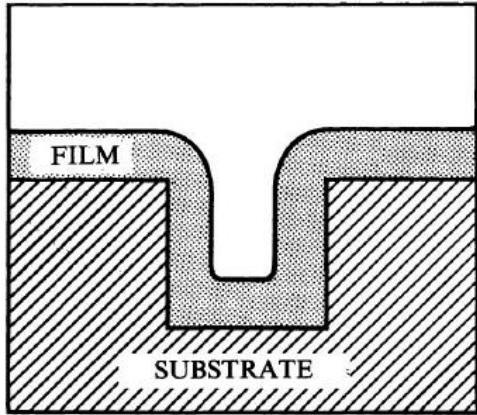
A low surface mobility

The PVD also gives columnar morphology.

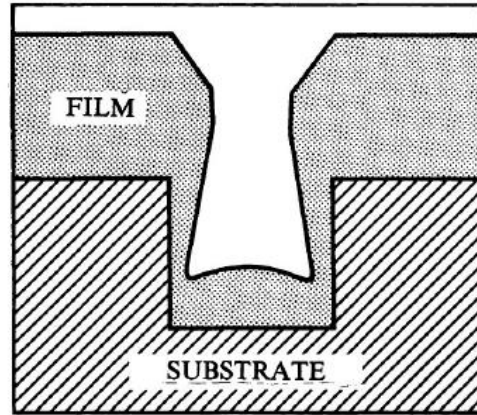
The high surface mobility of CVD growth results in a smooth conformal surface

## 2. The morphology of film growth

without argon dilution



with argon dilution



a trench cut in a substrate

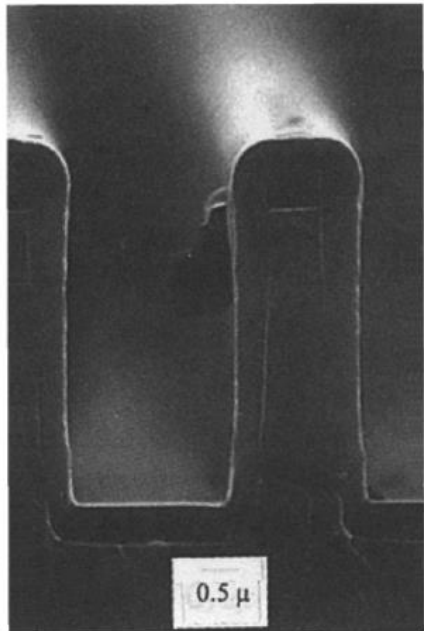
The flat, conformal, CVD-like growth

CVD with a low sticking coefficient

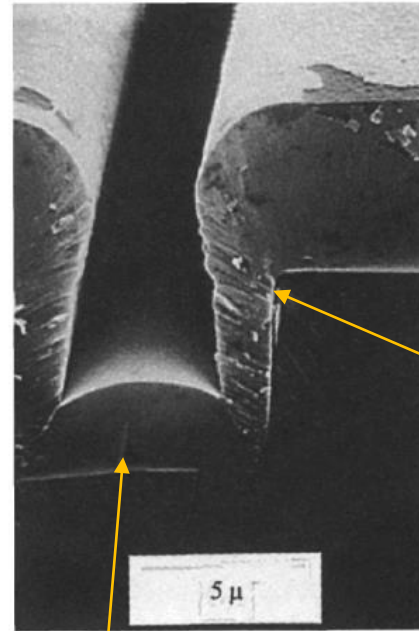
the growth is partially limited by the flux to the surface, a PVD process

PVD films: high density of electronic defects, voids, rapid oxidation

CVD films: lower defect density, a thin layer of oxidation on the surface



(a)

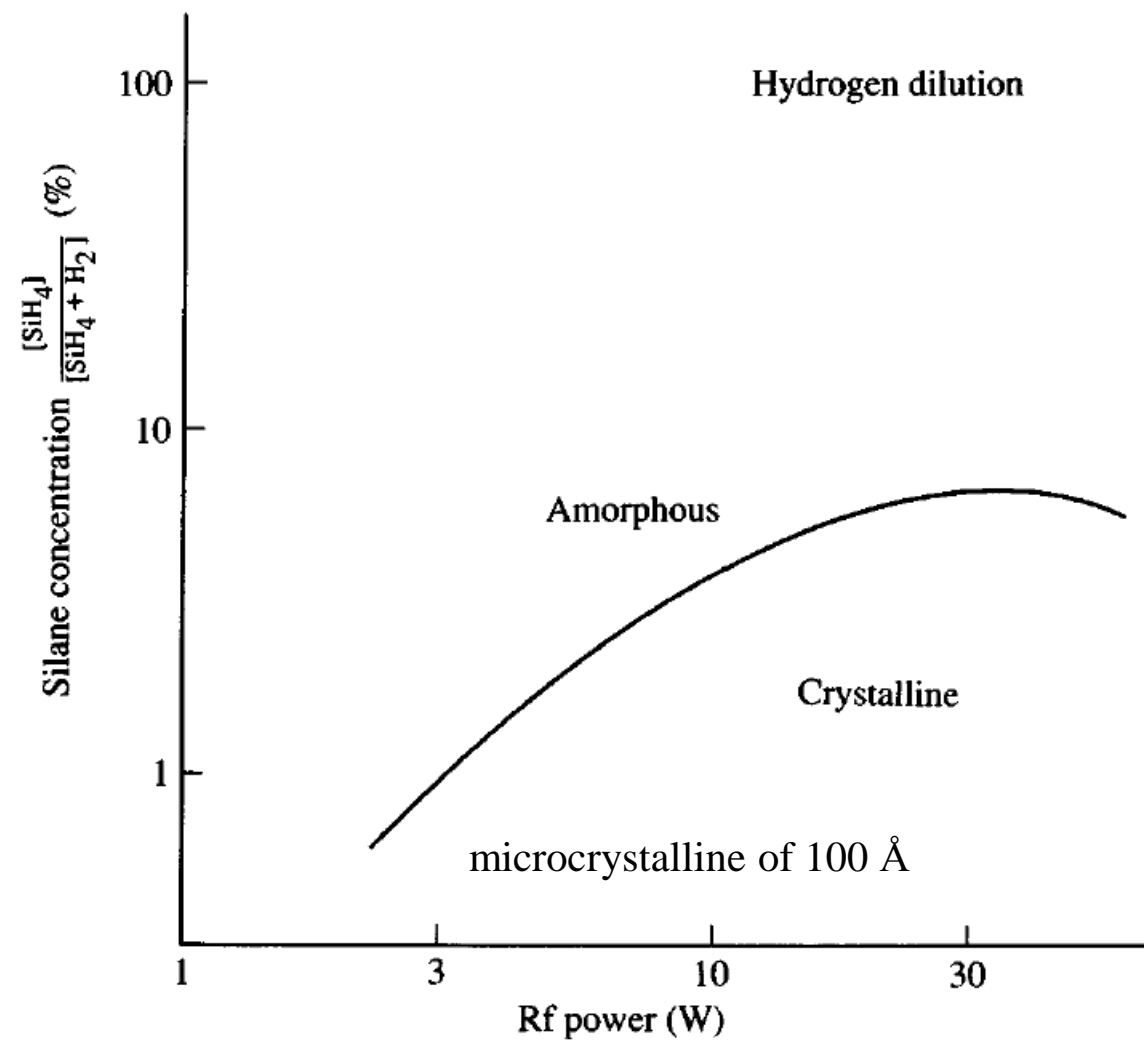
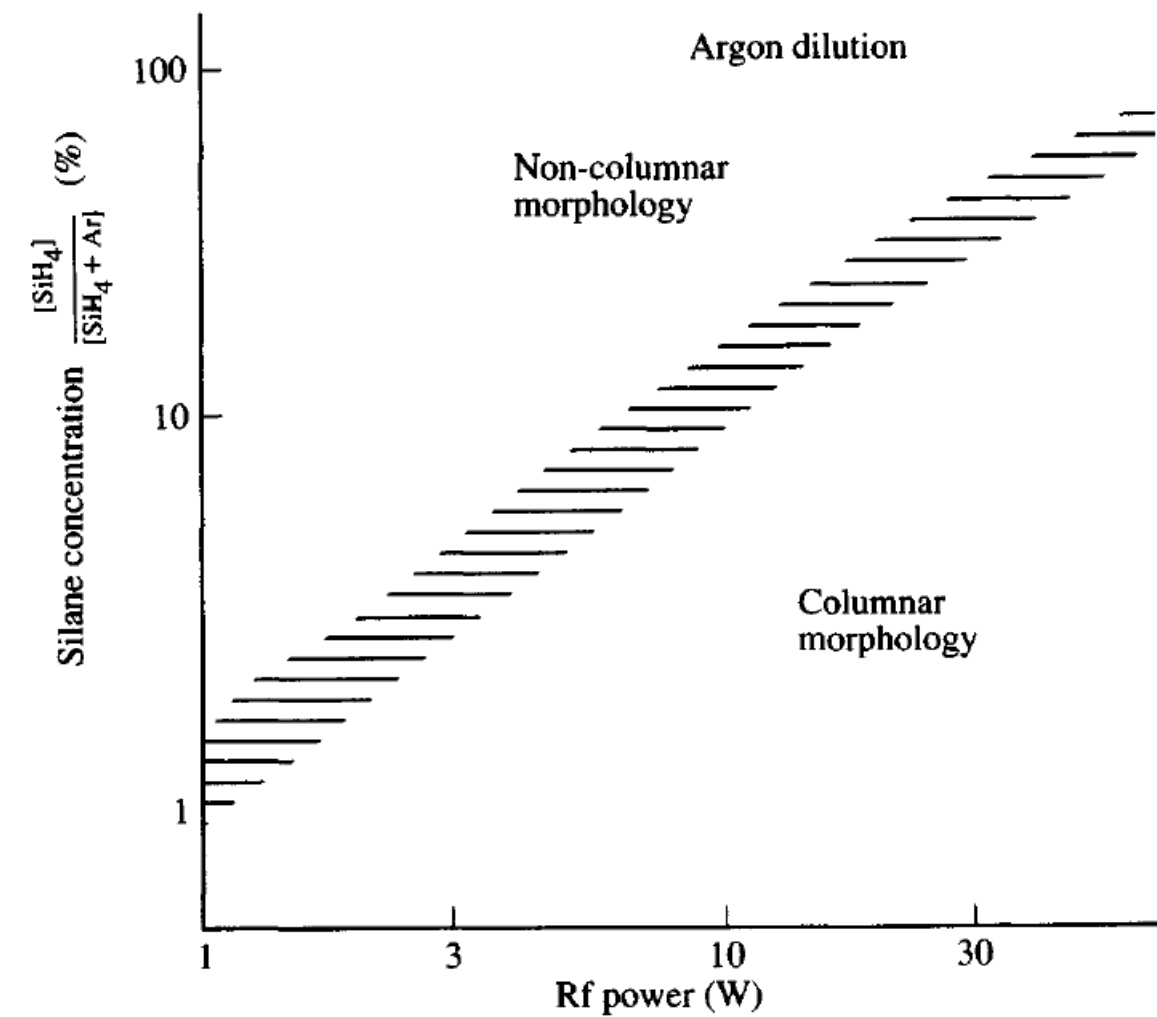


(b)

columnar structure

a pin-cushion shape

## 2. The morphology of film growth





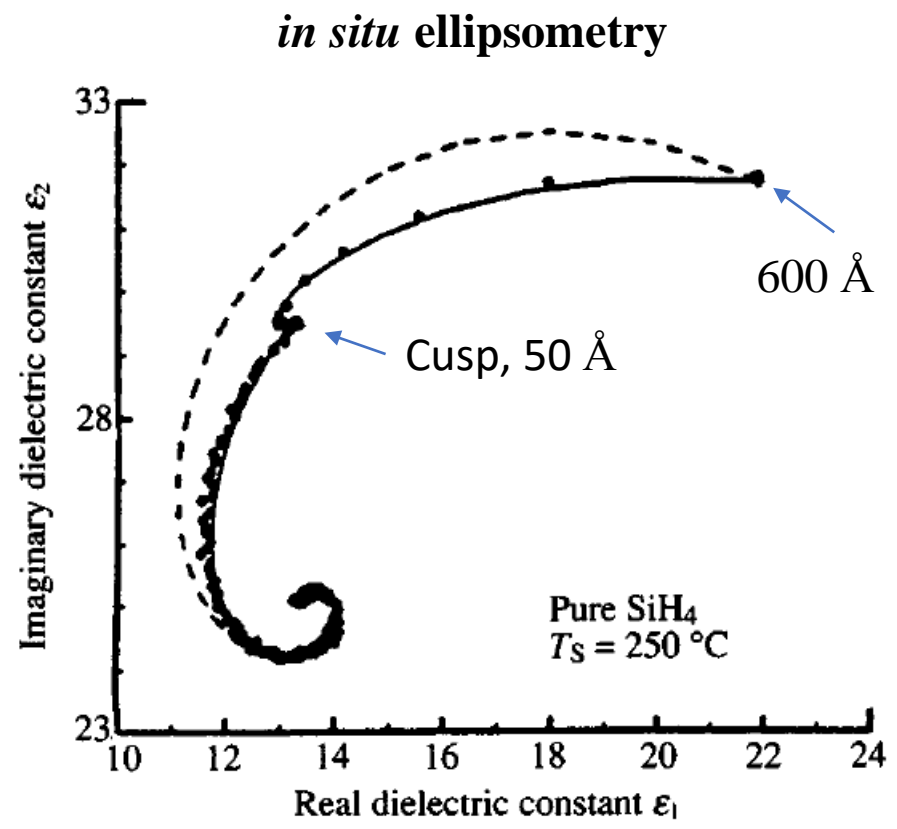
## 2. The morphology of film growth

The structure and morphology of the a-Si:H films obviously depend greatly on the form of the growing surface

In situ pseudo-dielectric function data at 3.4 eV (points) for the growth of intrinsic a-Si:H from pure SiH<sub>4</sub> at 250 °C on c-Si substrates.

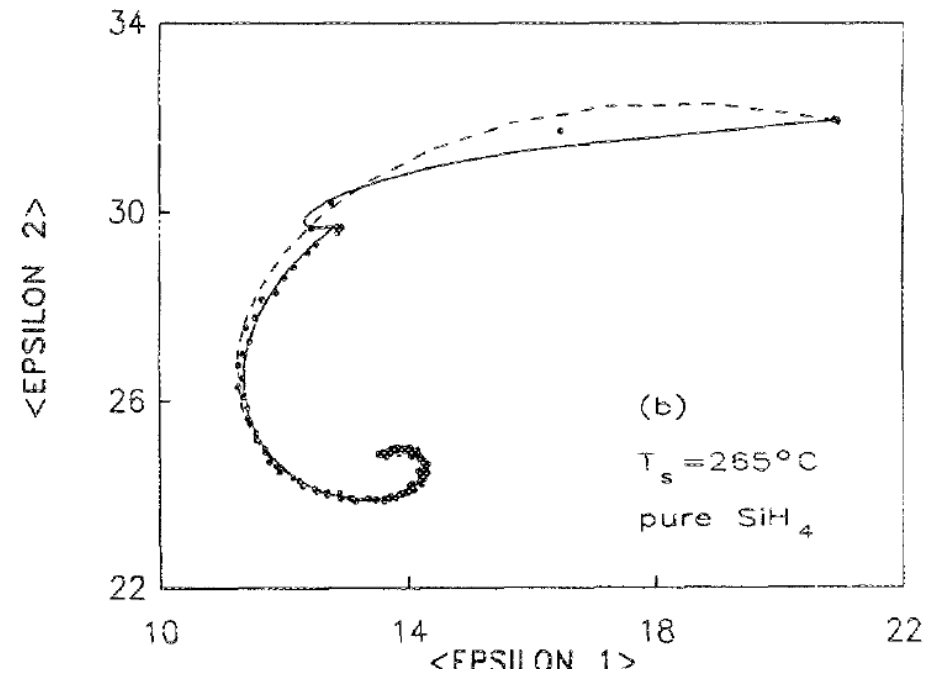
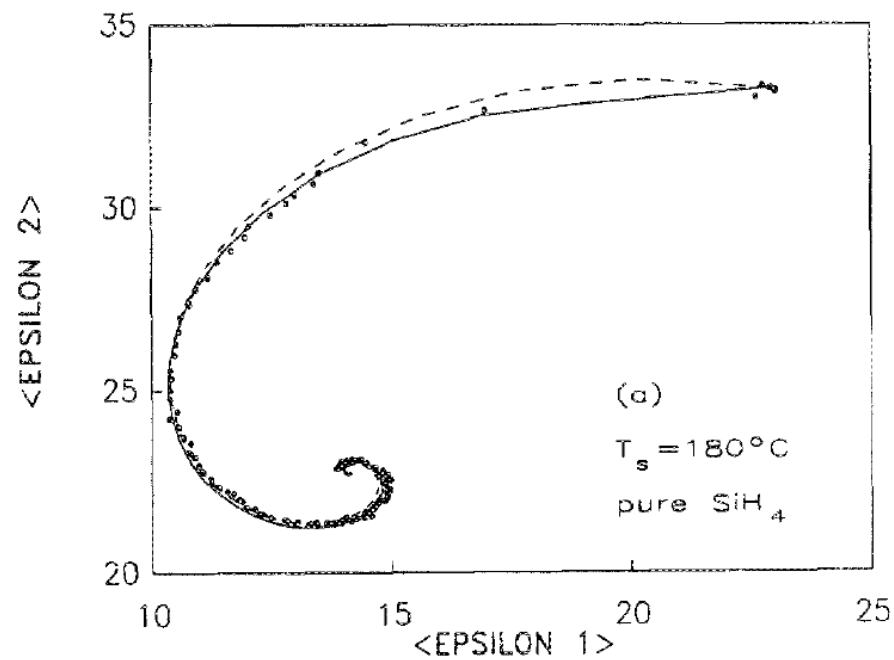
A two-step initial microstructure formation and coalescence sequence.

The cusp structure results from non-uniform nucleation of the film

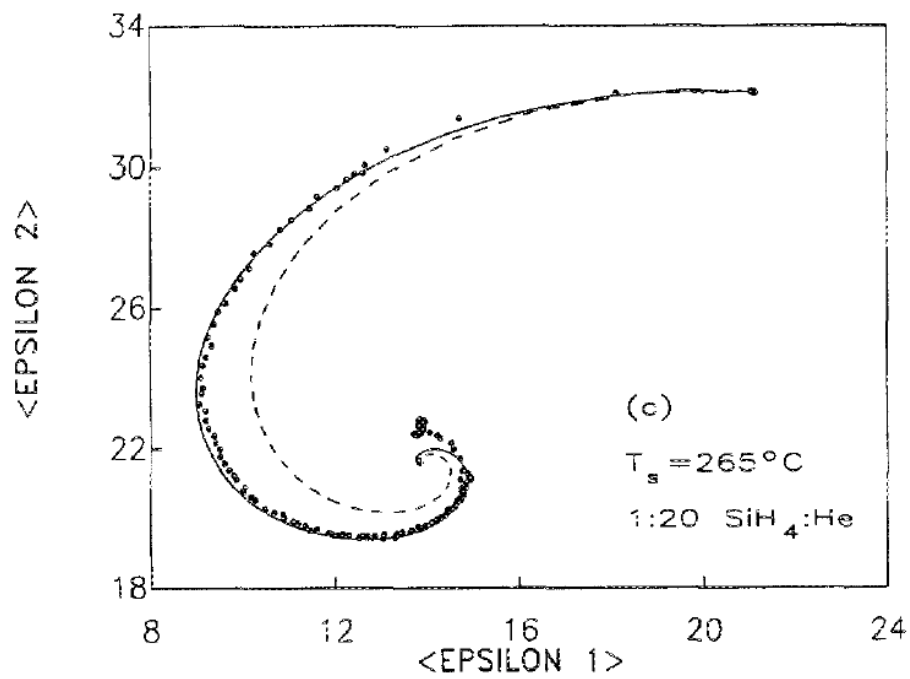
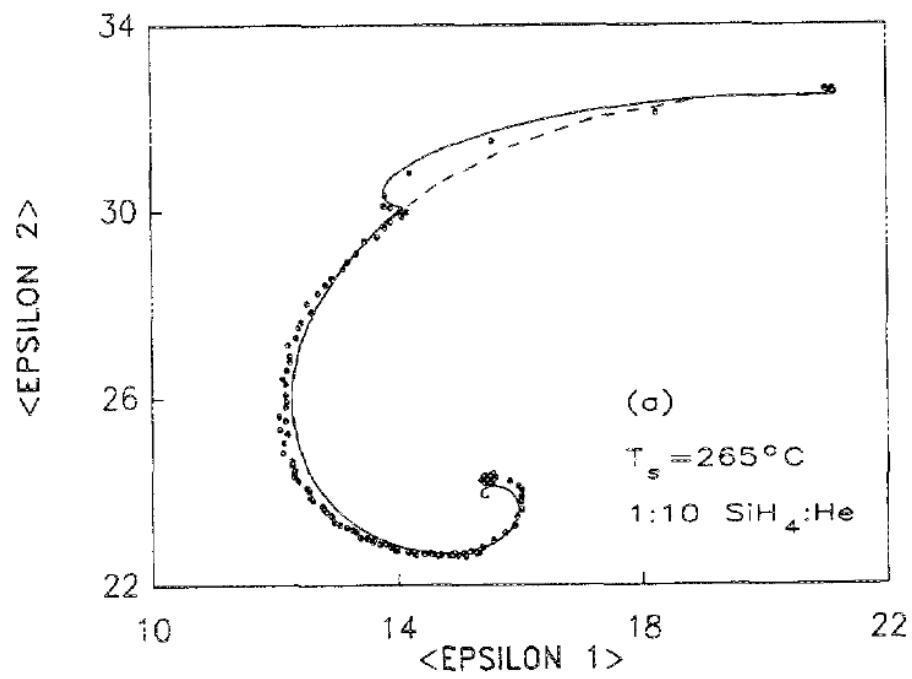


Predicted trajectory for uniform growth (dashed) and island growth (solid)

## 2. The morphology of film growth



No cusp due to low surface mobility suppressing the island formation



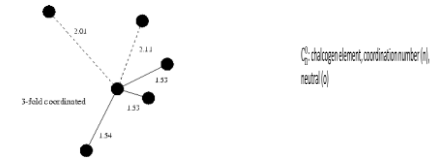
No cusp due to a columnar microstructure which continues through the film

THANK YOU!  
Any questions?

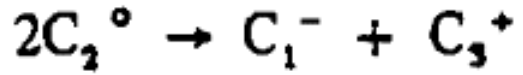


# Defects reaction

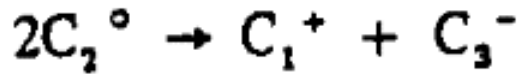
three-fold coordinated



$C_n^o$ : chalcogen element, coordination number (n), neutral (o)



Defect formation energy:  $U_{LP}$



Defect formation energy:  $E_b + 2\Delta + U_{\sigma^*}$

defect pairs  $C_1^- + C_3^+$  which they designate as valence alternation pairs (VAPs) are frozen into the structure at the temperature of the glass transition  $T_g$

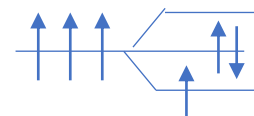
Defect formation energy:  $E_b + 2\Delta + U_{\sigma^*}$

The number of these defects,  $N_D$  is then given by

$$N_D = N_O \exp(-U_{LP}/2kT_g) \quad U_{LP} \text{ is small, } \sim 0.8 \text{ eV}$$

$N_O$  is the total number of chalcogen atom sites.

$C_1^+$



$-E_b$

## Defects reaction

defect pairs  $C_1^- + C_3^+$  which they designate as valence alternation pairs (VAPs) are frozen into the structure at the temperature of the glass transition  $T_g$

The number of these defects,  $N_D$  is then given by

defect pairs  $C_1^- + C_3^+$  which they designate as valence alternation pairs (VAPs) are frozen into the structure at the temperature of the glass transition  $T_g$

$N_0$  is the total number of chalcogen atom sites.

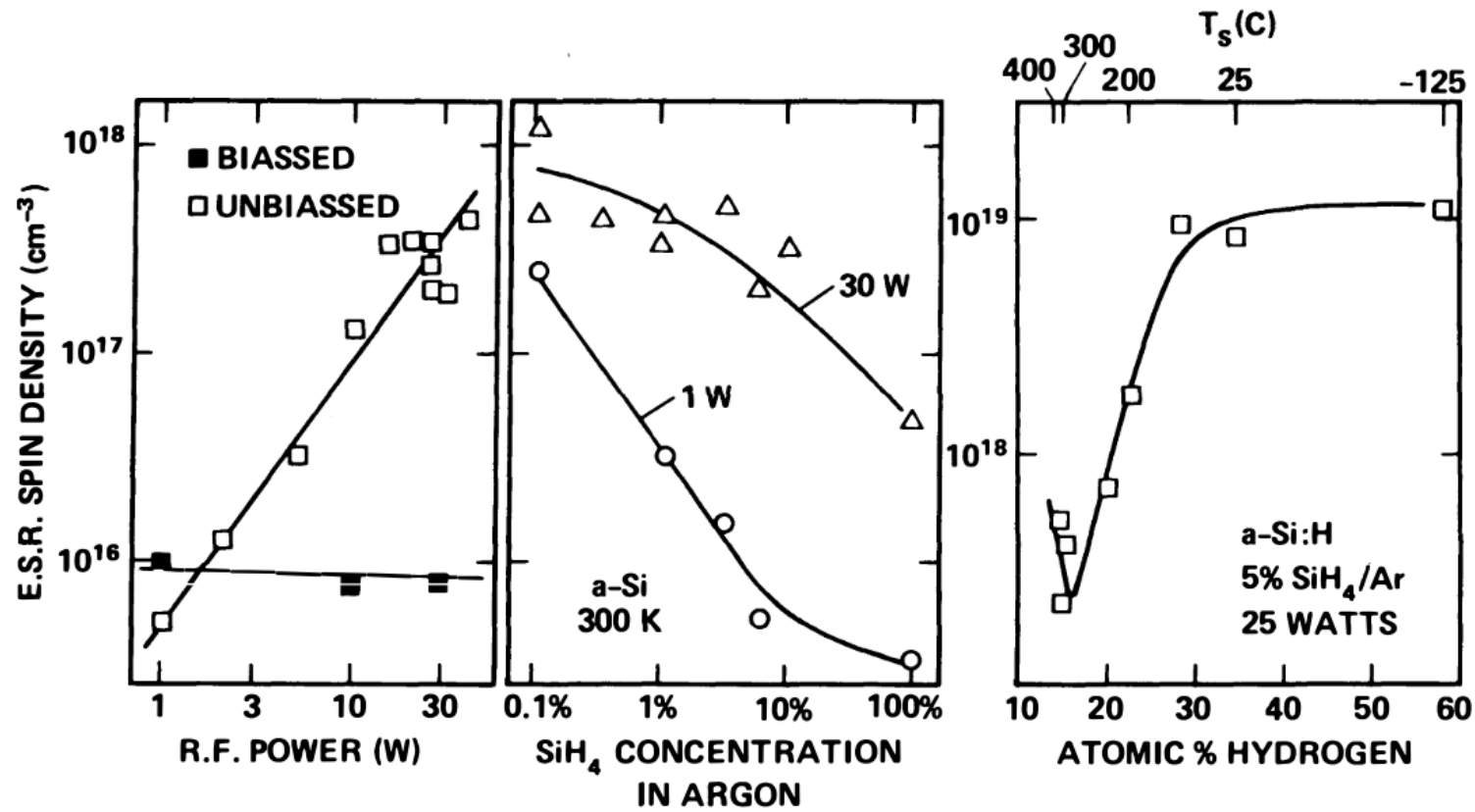


Fig. 10. Electron spin density in a-Si: H (a) as a function of RF power; (b) as a function of silane concentration; (c) as a function of H $_2$  content (obtained by varying  $T_s$ ).