



Aalto University  
School of Chemical  
Technology

# CHEM E5125 Thin Film Technology

## Lecture 3 PVD 1

### Plasma and ion bombardment

Jari Koskinen

[jari.koskinen@aalto.fi](mailto:jari.koskinen@aalto.fi)

19.1.2021

# Contents

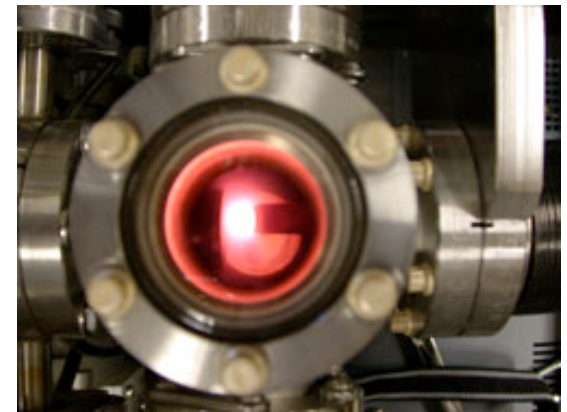
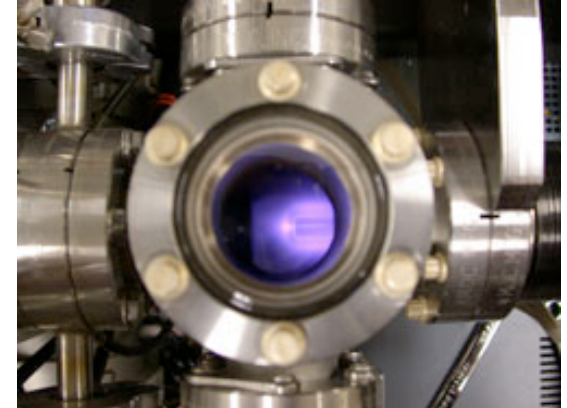
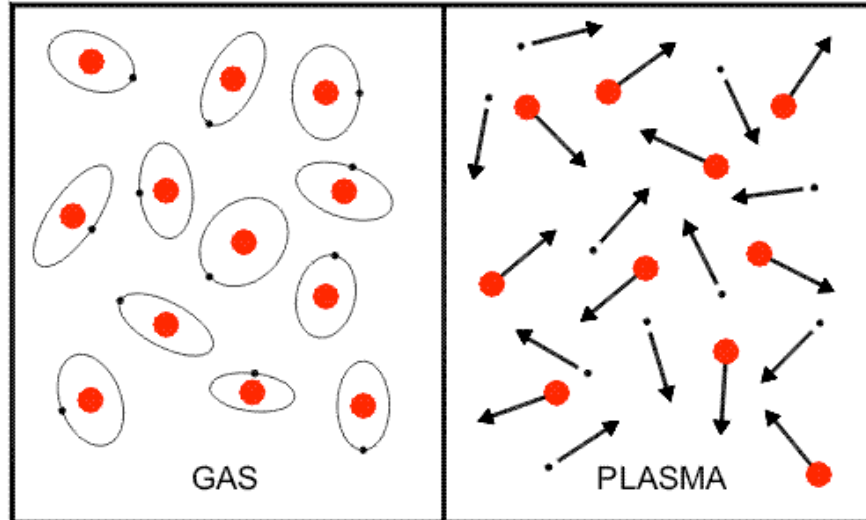
- Plasma types
- Generation of plasma
- Ion solid interaction
- Thin film microstructure in PVD



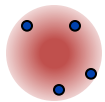
# Plasma

- Plasma

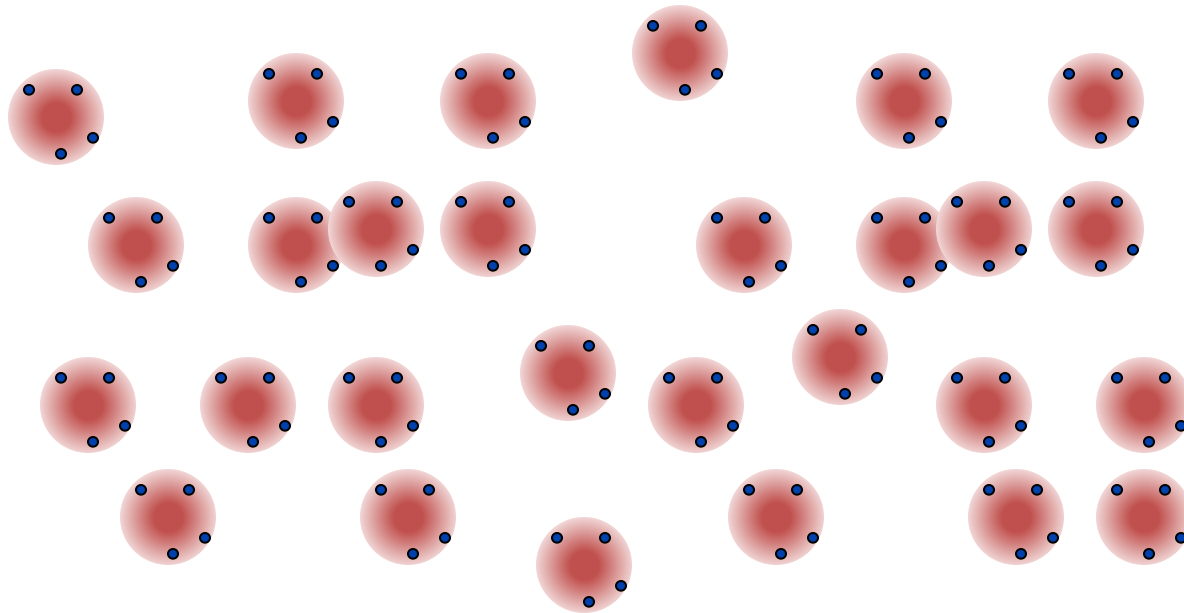
- Gas of positive ions, electrons and (mostly) neutral atoms
- Etymology: Greek: “moulded” - plasma fills the chamber
- Charge neutrality  $n_e = n_i$
- Colliding electrons ionise atoms
- Ions and electrons accelerate in electric field
- Collisions excite atoms



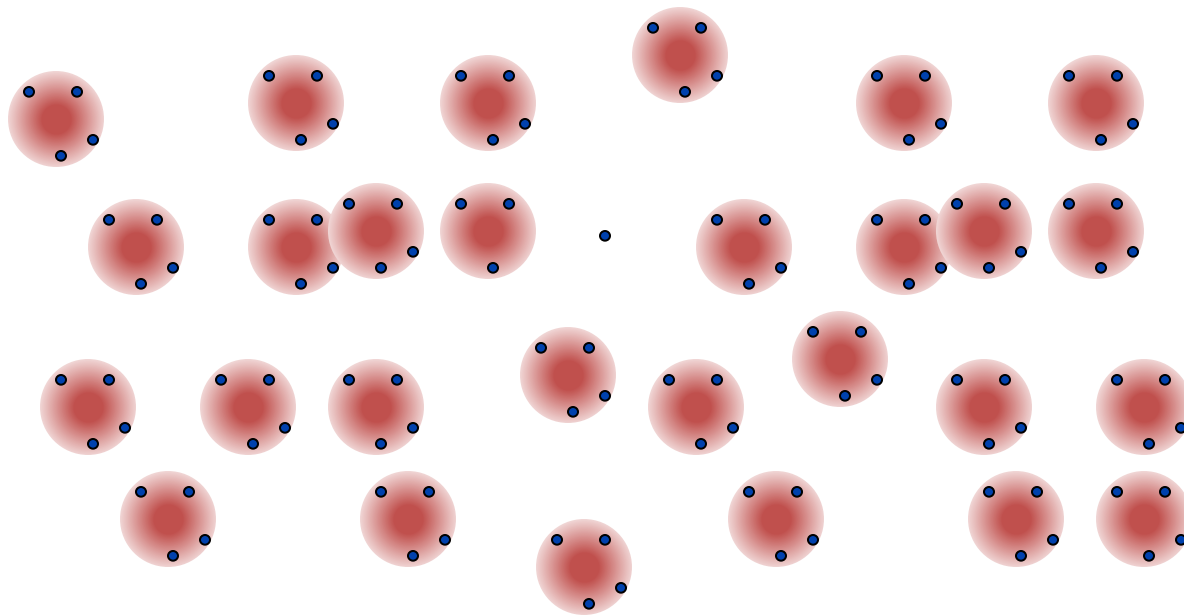
# Glow discharge



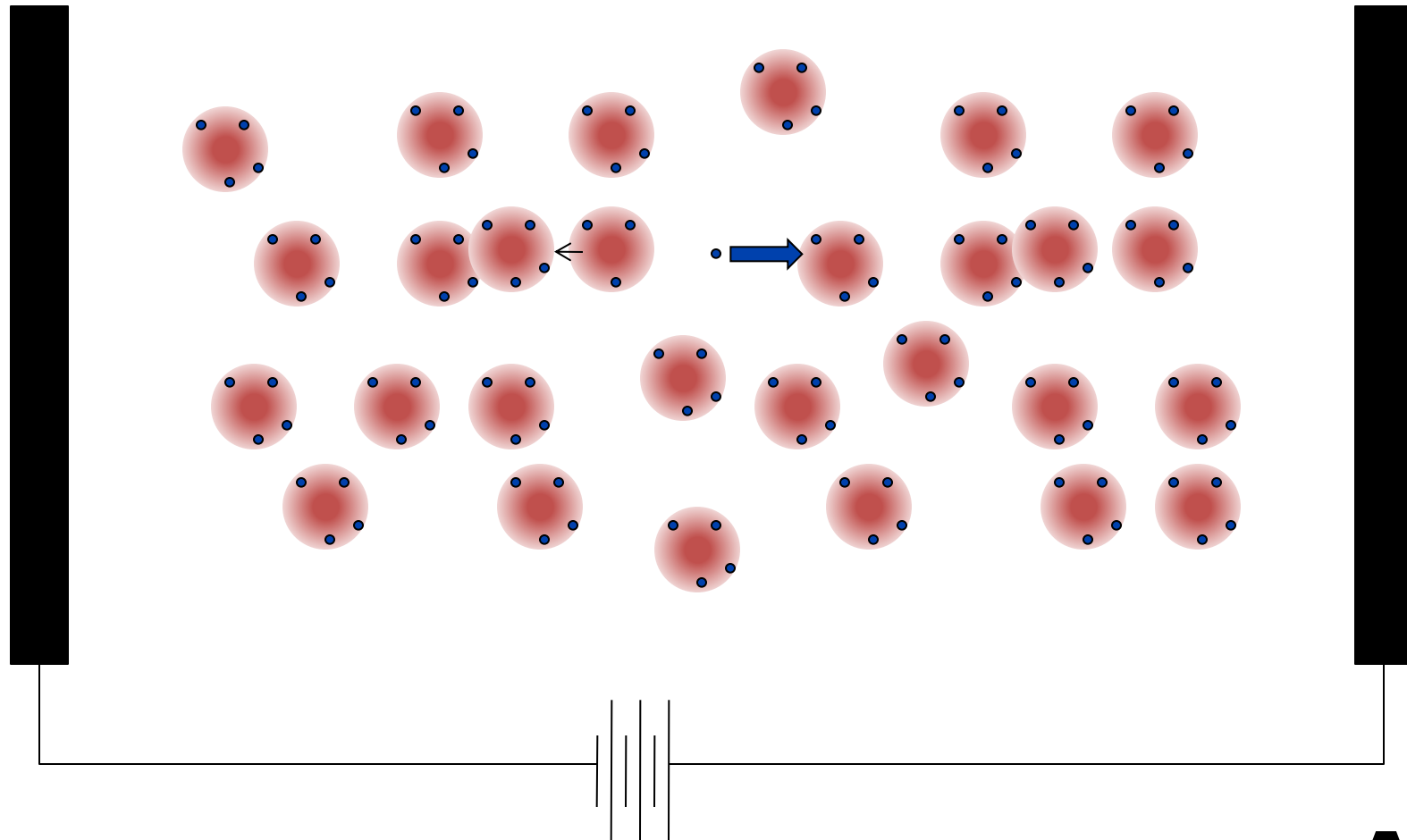
# Glow discharge



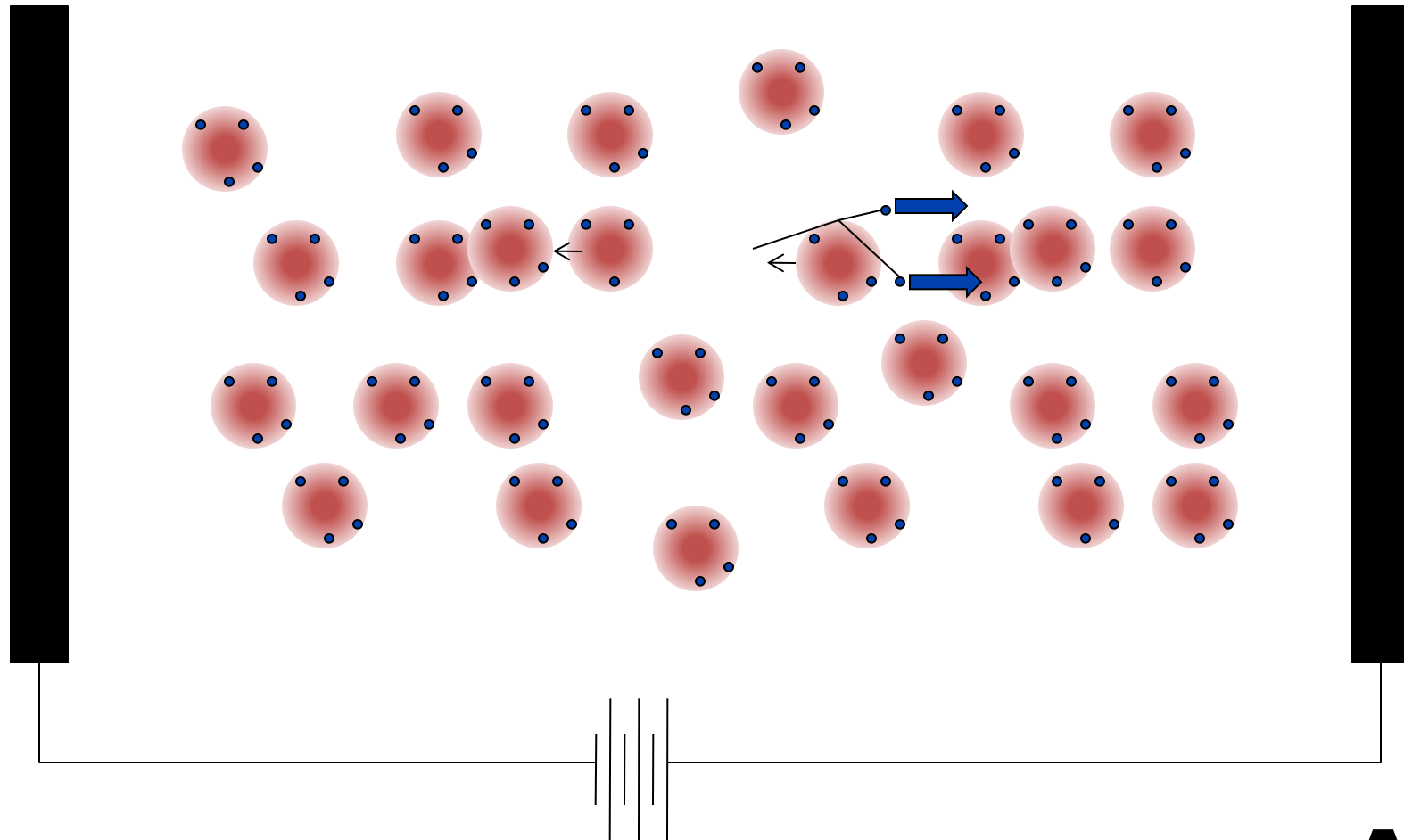
# Glow discharge



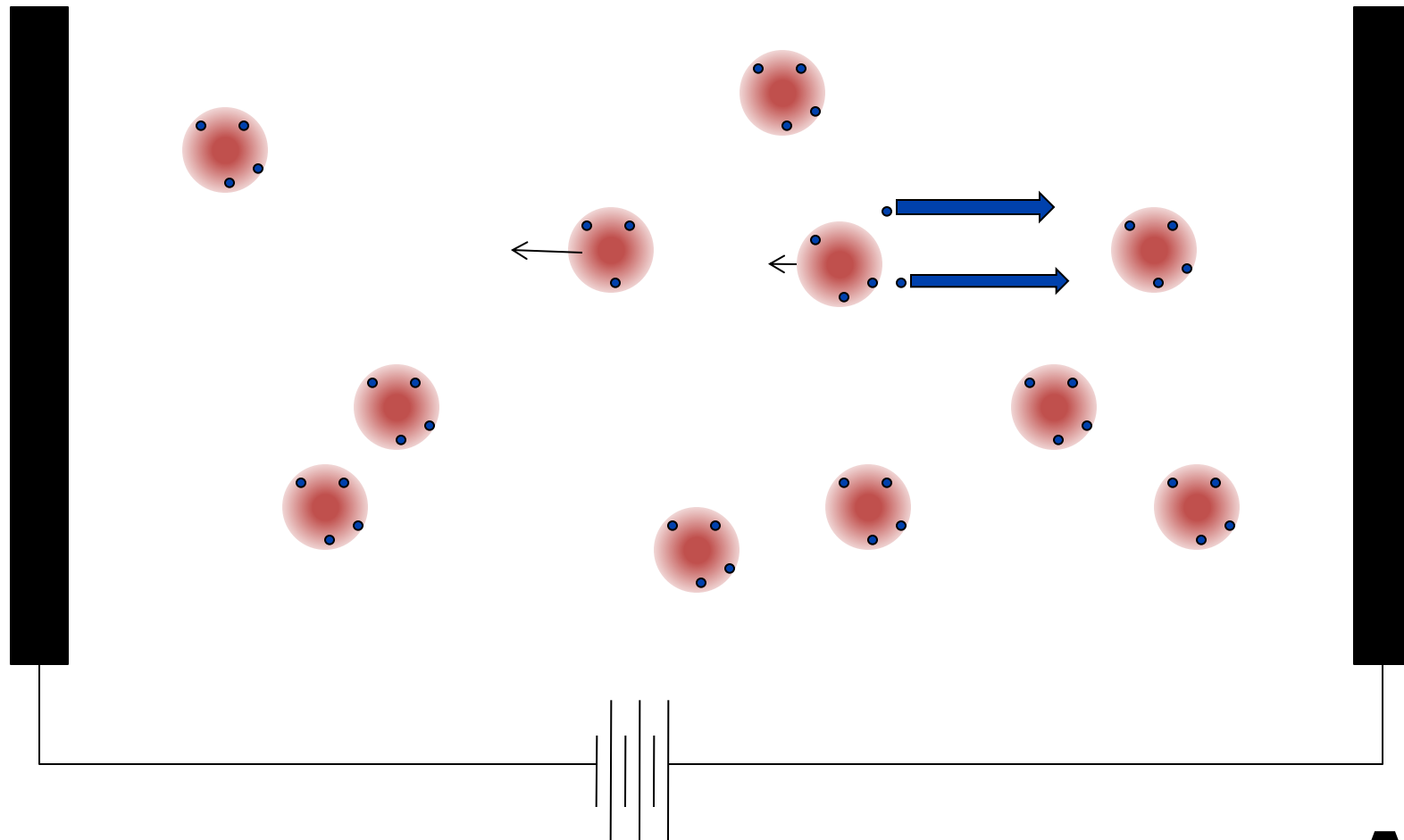
# Glow discharge



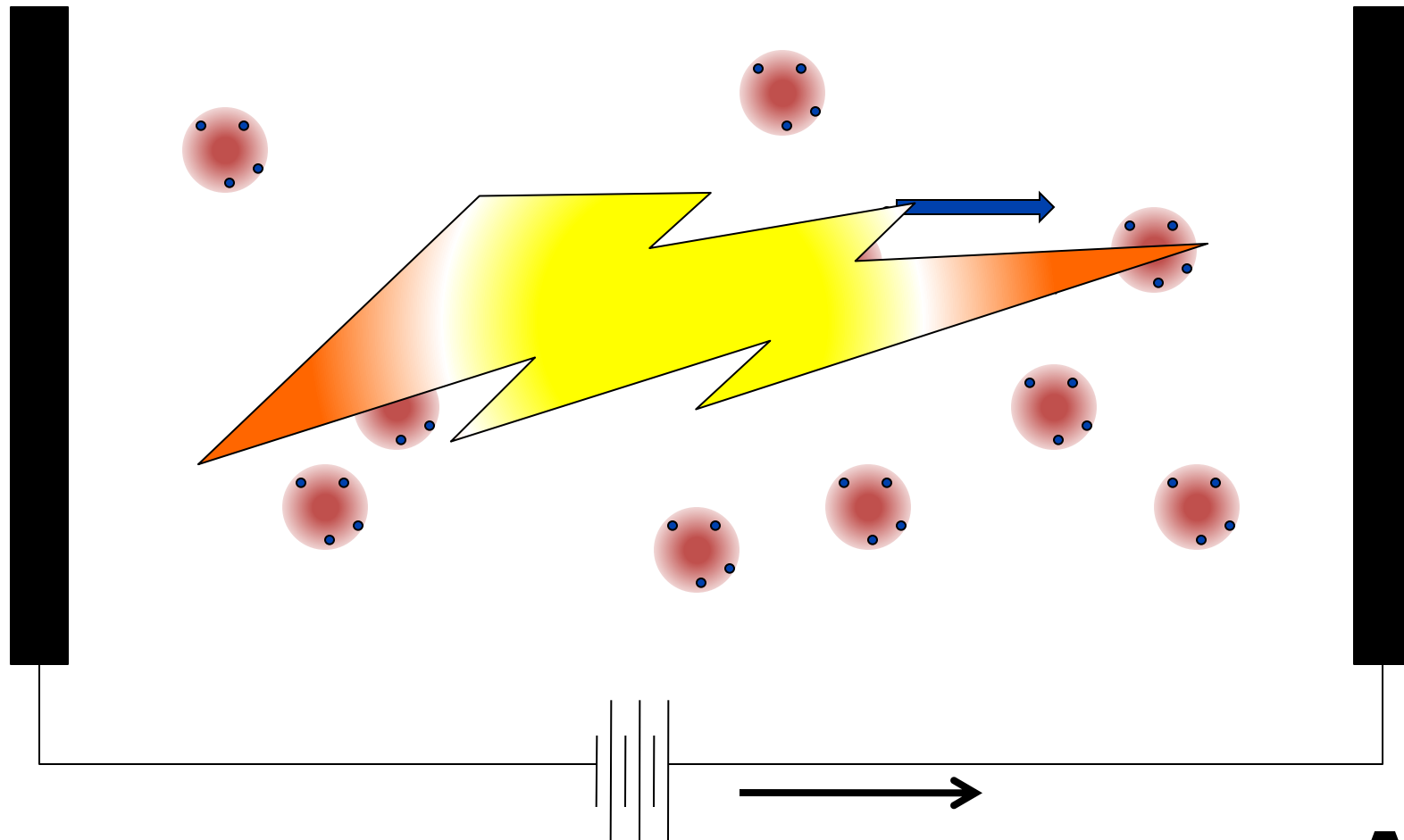
# Glow discharge



# Glow discharge

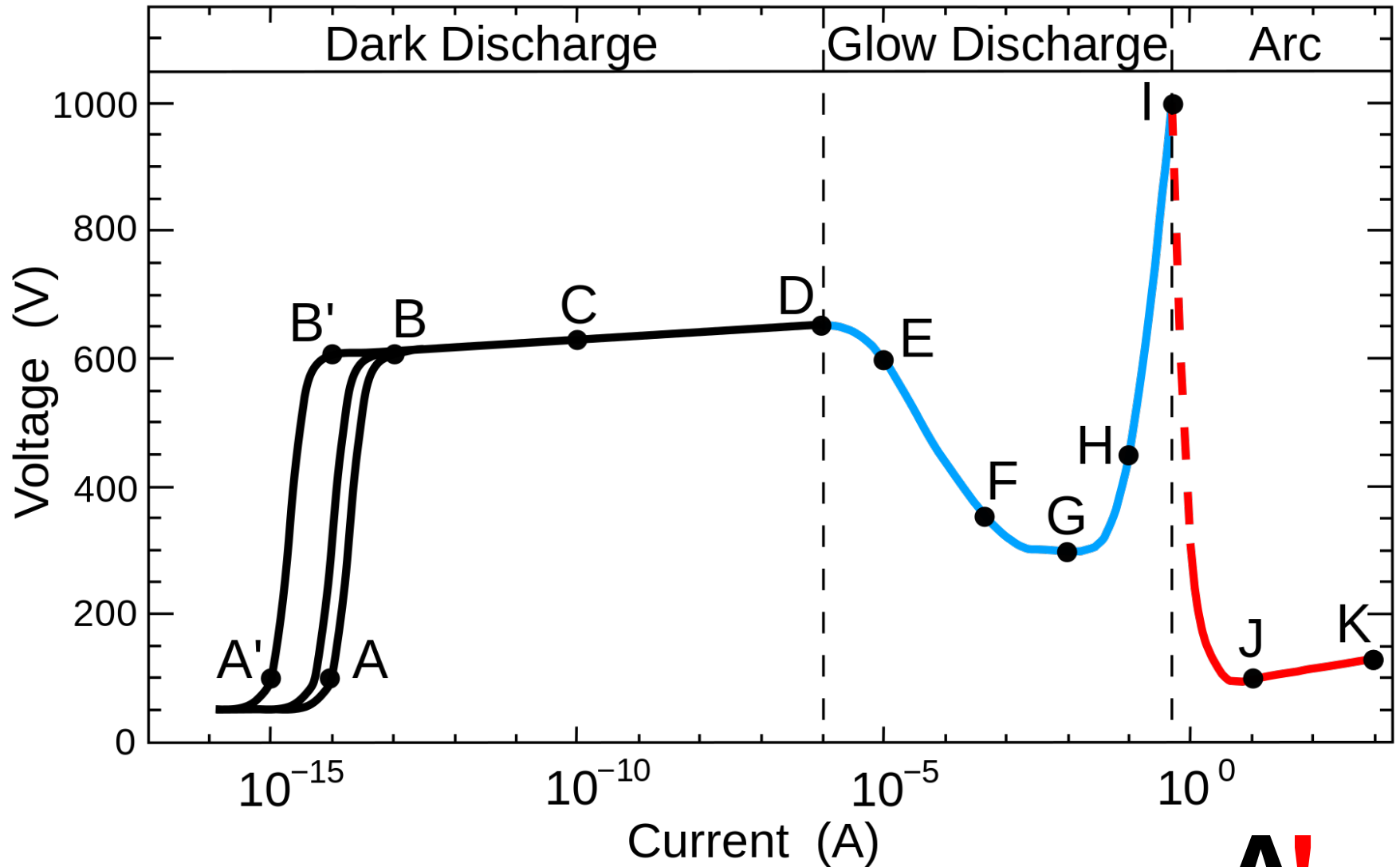


# Glow discharge

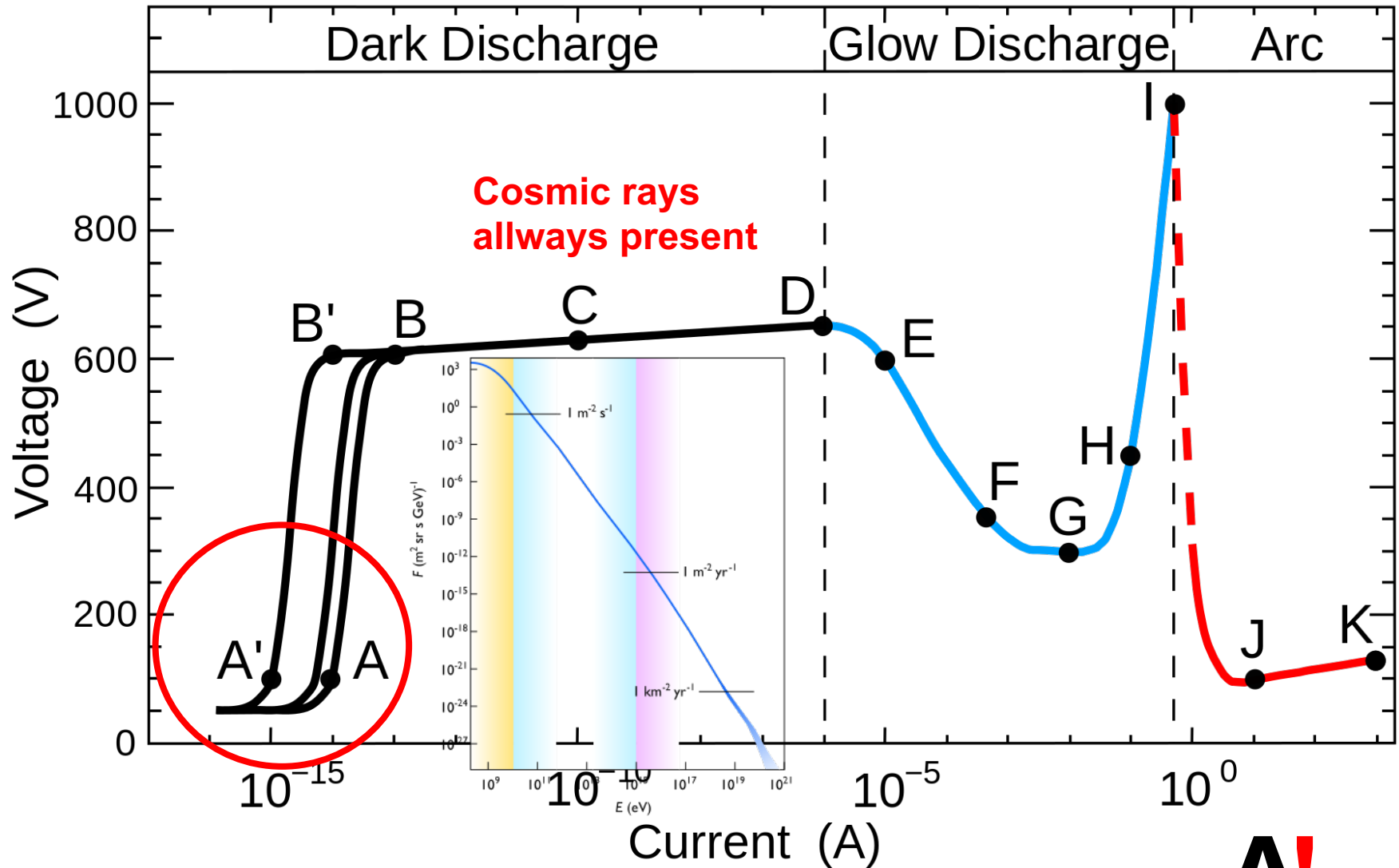




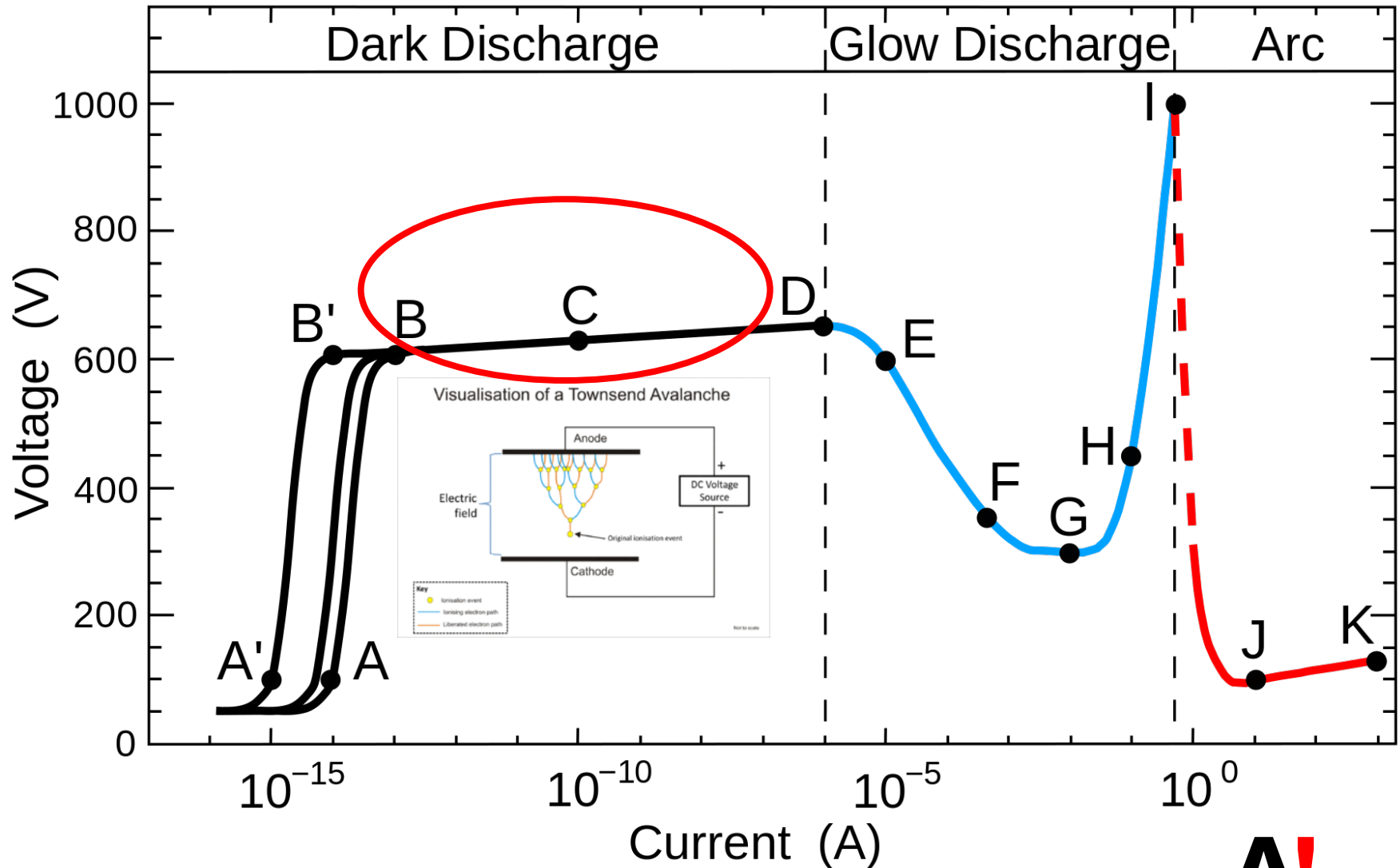
# DC Plasma glow discharge and arc



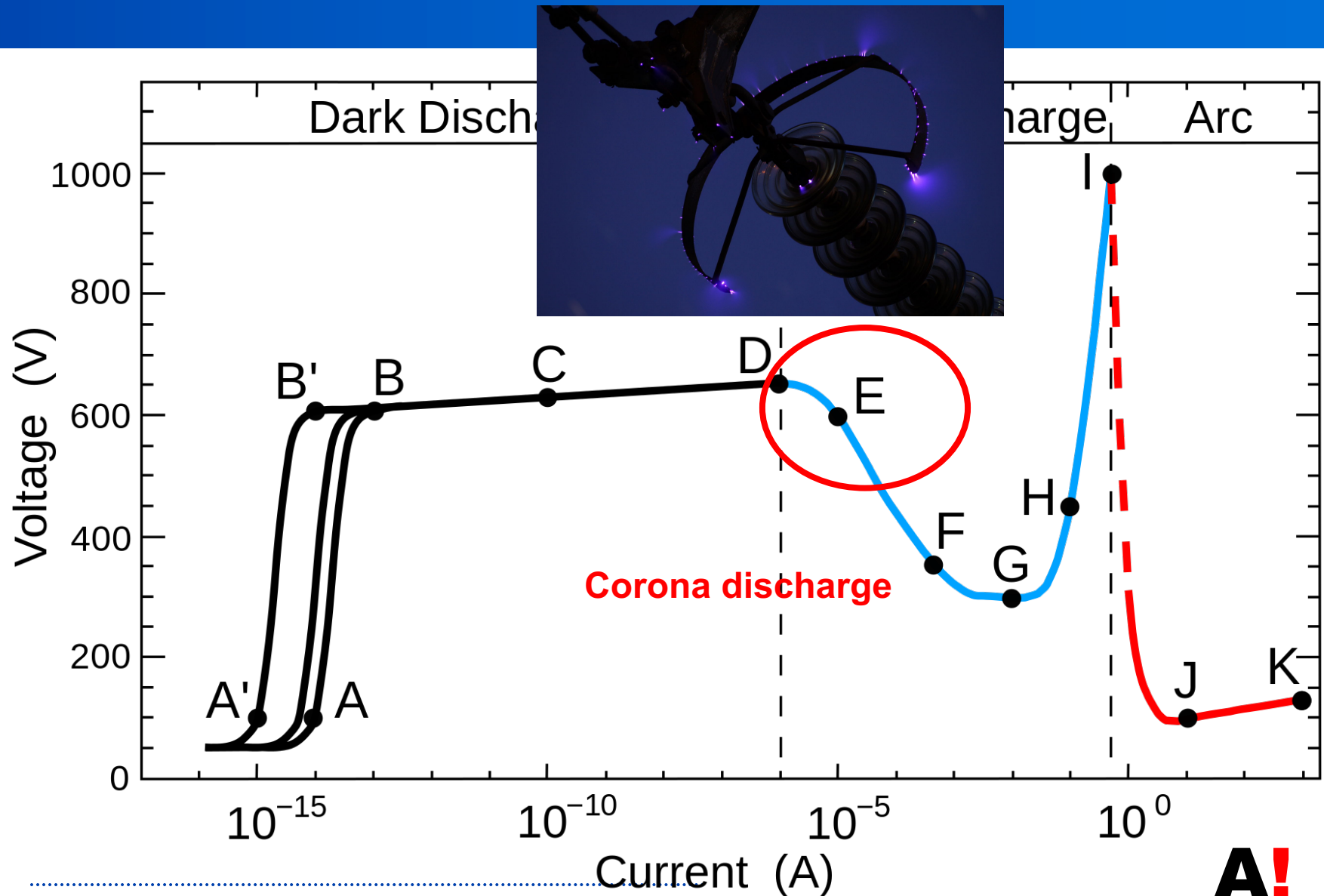
# DC Plasma glow discharge and arc



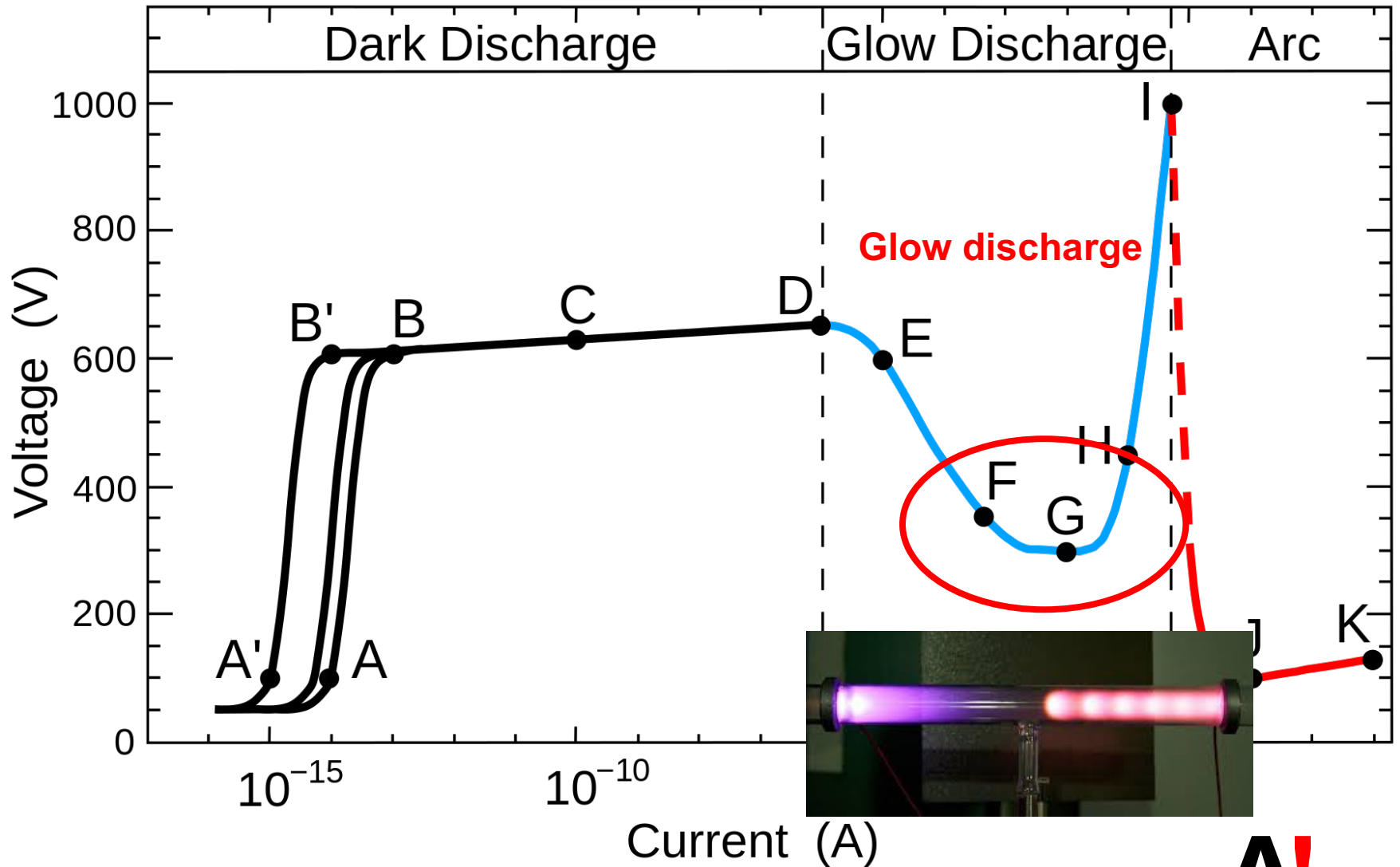
# DC Plasma glow discharge and arc



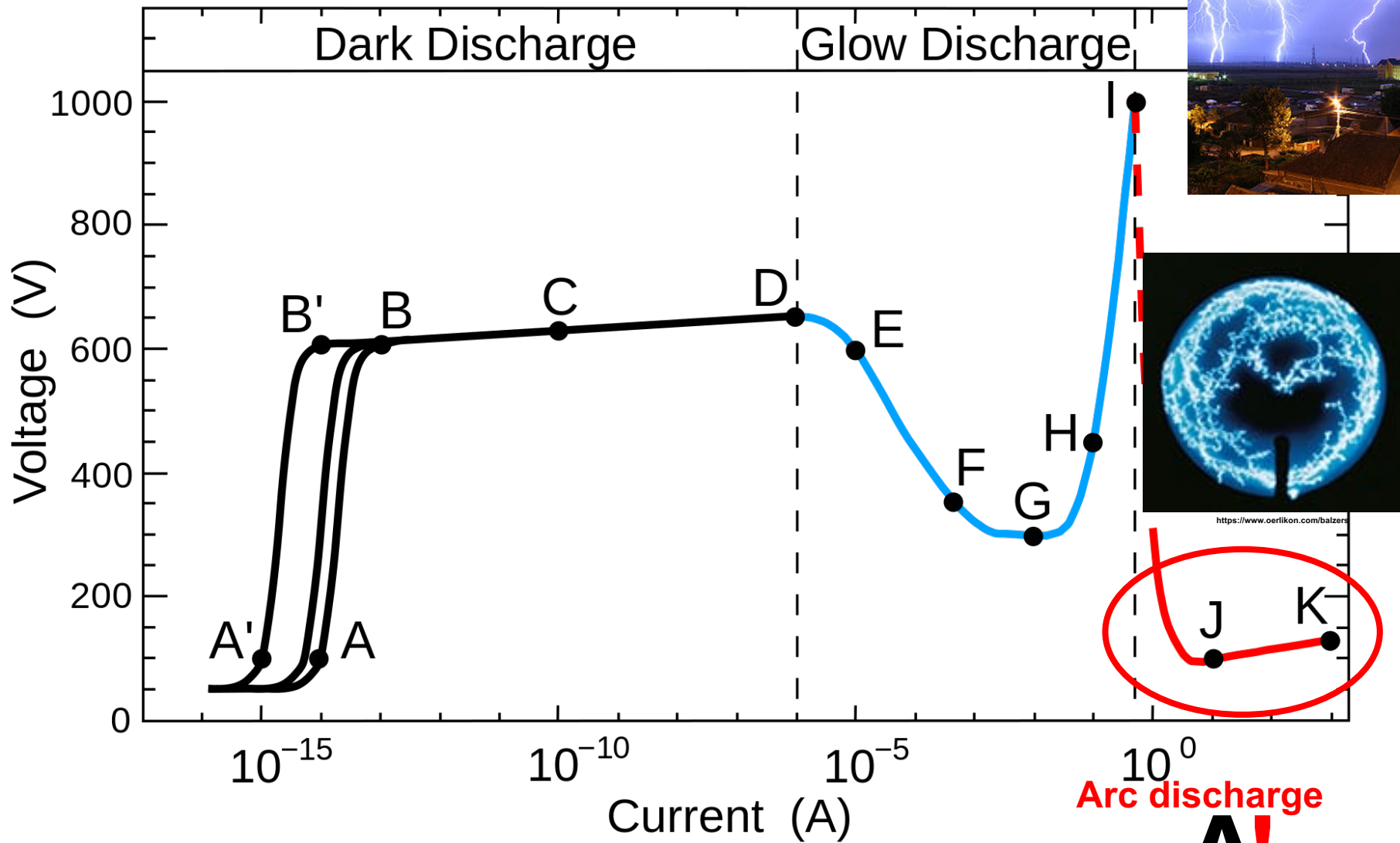
# DC Plasma glow discharge and arc



# DC Plasma glow discharge and arc



# DC Plasma glow discharge and arc



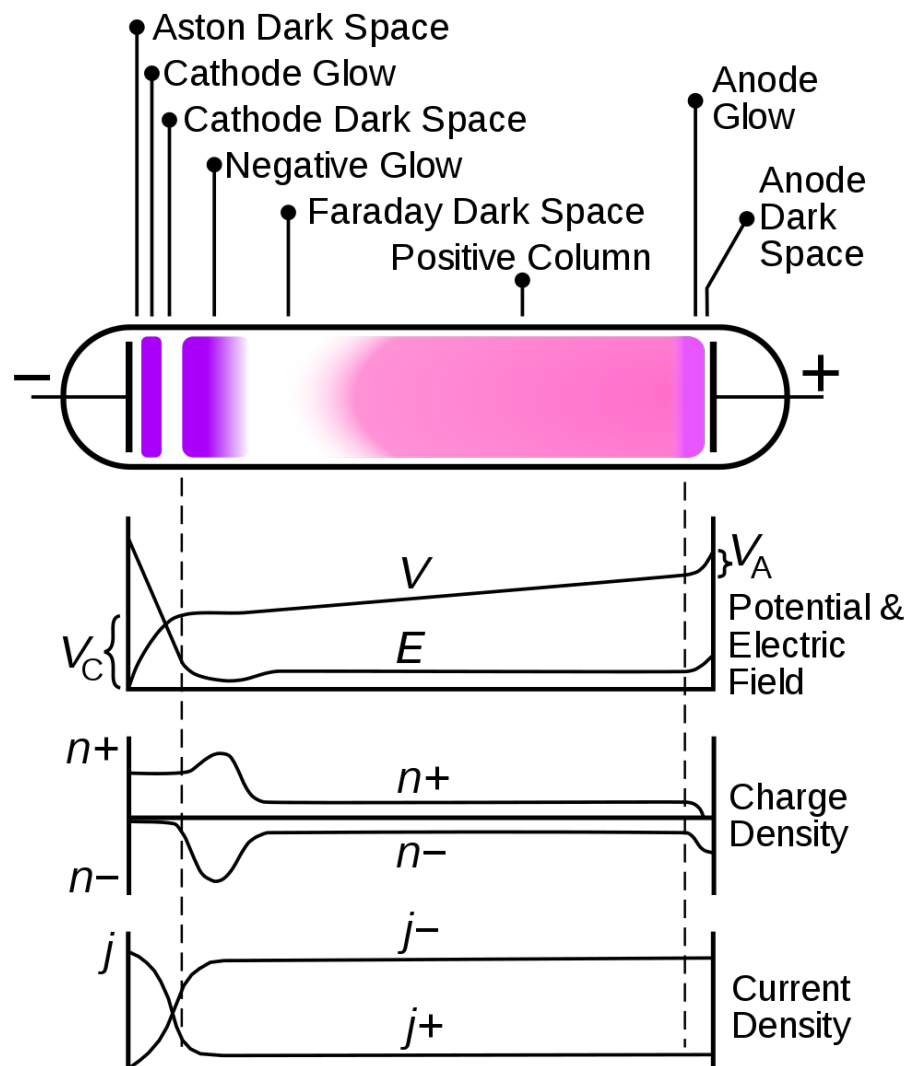
<https://www.oerlikon.com/balzern>

Arc discharge

**A!**

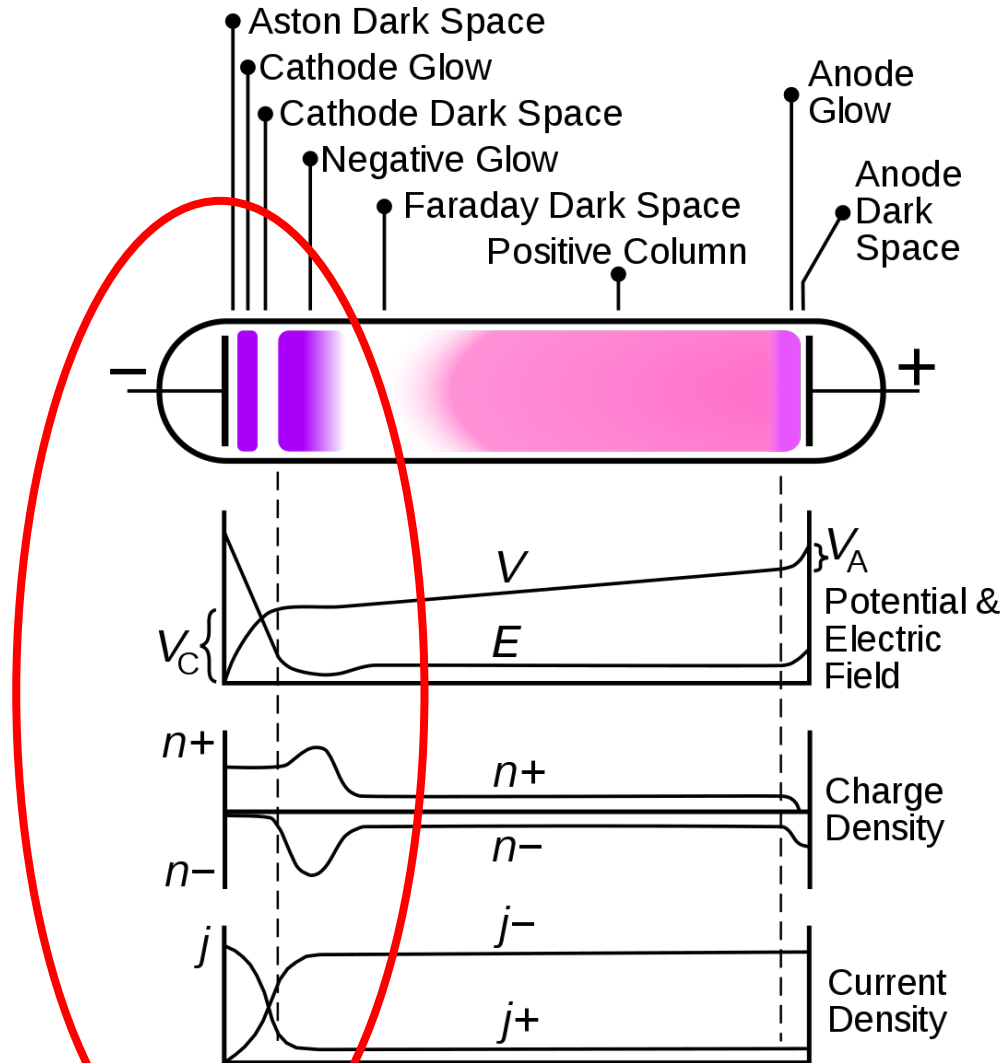
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# Glow discharge plasma



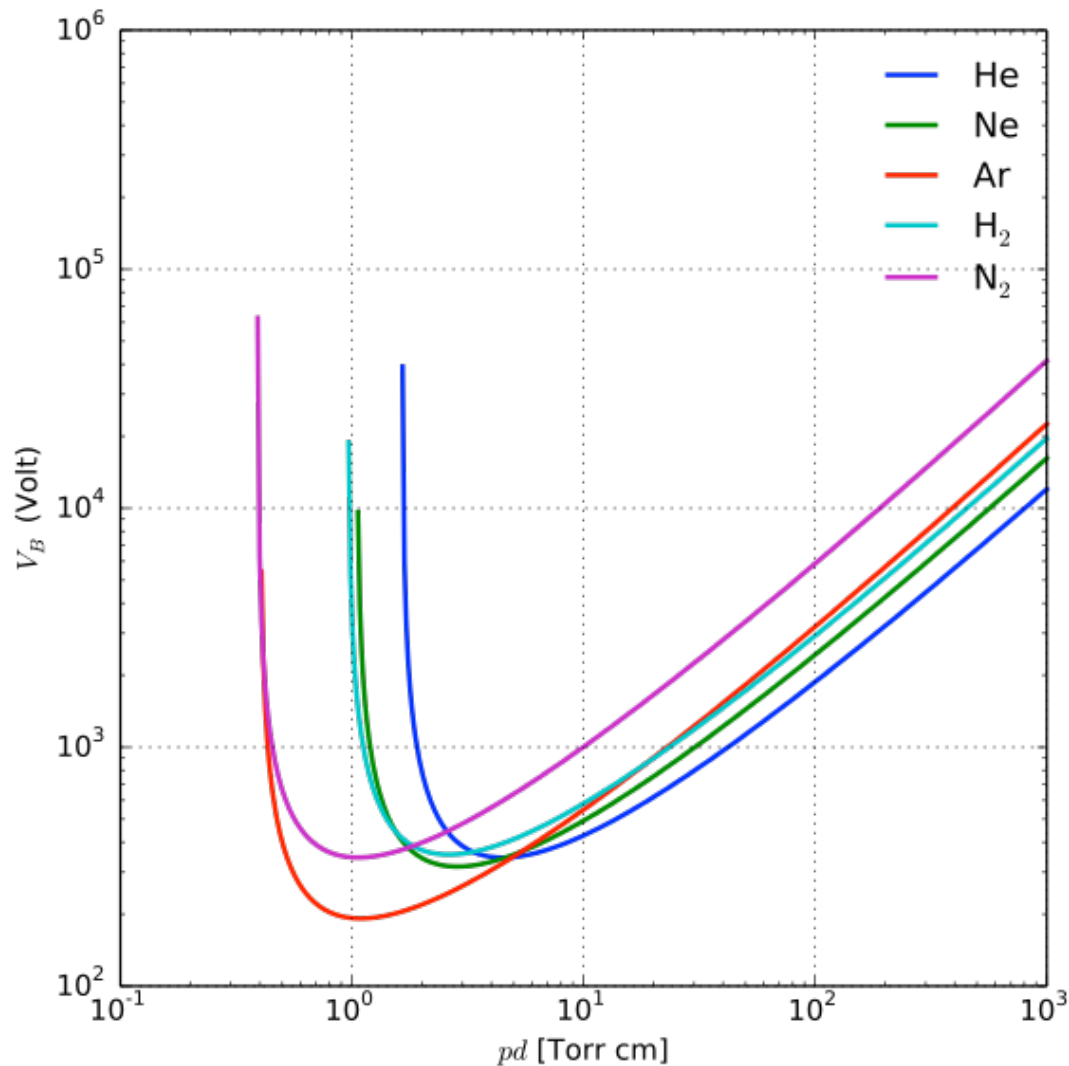
# Glow discharge plasma

For PVD  
Interesting things  
happen  
here

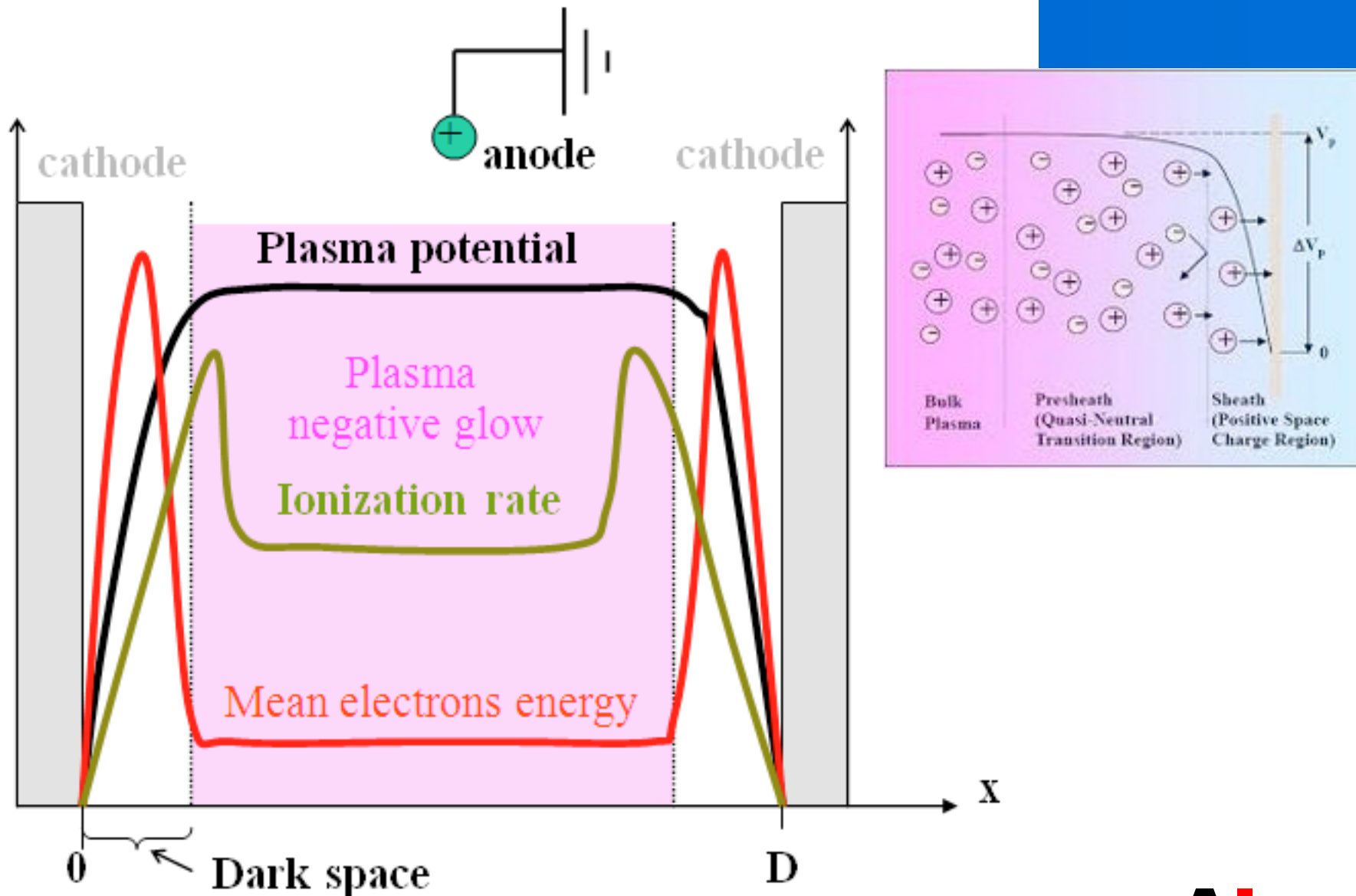




# Breakdown voltage Paschen minimum



# DC plasma



# Important plasma parameters

- Oscillations
- Debye length
- mean free path
- ionization crosssection

# Plasma oscillation

Assume:  $n_0$  fixed ions (+) &  $n_0$  moving electrons (-)

Apply a small electric field  $\mathbf{E}_1$

$$n_+ = n_0$$

→ electrons move:

$$n_- = n_0 + n_1(\mathbf{r}, t) ; n_1 \ll n_0$$

Electron continuity equation:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}) = 0$$

$$n = n_0 + n_1(\mathbf{r}, t) ; \mathbf{u} = \mathbf{u}_0 + \mathbf{u}_1(\mathbf{r}, t) \quad (\mathbf{u}_0 = 0 \leftrightarrow \text{electrons are assumed cold})$$

$$\frac{\partial n_0}{\partial t} + \frac{\partial n_1}{\partial t} + \nabla \cdot ((n_0 + n_1)\mathbf{u}_1) = 0 \Rightarrow \frac{\partial n_1}{\partial t} + n_0 \nabla \cdot \mathbf{u}_1 + \nabla \cdot (n_1 \mathbf{u}_1) = 0$$

0 2<sup>nd</sup> order

Linearized continuity equation (1st order terms only):  $\frac{\partial n_1}{\partial t} + n_0 \nabla \cdot \mathbf{u}_1 = 0$  !!

Force:  $\mathbf{F} = q\mathbf{E} \Rightarrow m_e \frac{\partial \mathbf{u}_1}{\partial t} = -e\mathbf{E}_1$

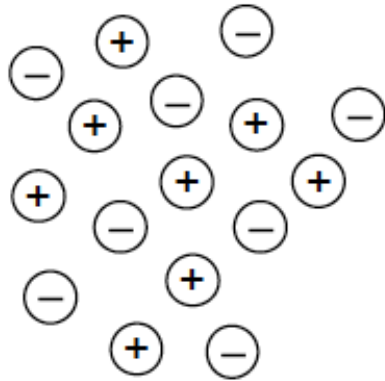
1st Maxwell:  $\nabla \cdot \mathbf{E}_1 = -en_1/\epsilon_0$

$$\Rightarrow \frac{\partial^2 n_1}{\partial t^2} + \left( \frac{n_0 e^2}{\epsilon_0 m_e} \right) n_1 = 0$$

$$\omega_{pe}^2 = \frac{n_0 e^2}{\epsilon_0 m_e}$$

plasma frequency

# Debye screening



Coulomb potential of each charge:

$$\varphi = \frac{q}{4\pi\epsilon_0 r}$$

Assume thermal equilibrium (Boltzmann distribution)

$$n_\alpha(\mathbf{r}) = n_{0\alpha} \exp\left(-\frac{q_\alpha \varphi}{k_B T_\alpha}\right)$$

$\alpha$  labels the particle populations (e.g., e, p)

Introduce a test charge  $q_T$ . What will be its potential?

Home exercise: 
$$\varphi = \frac{q_T}{4\pi\epsilon_0 r} \exp\left(-\frac{r}{\lambda_D}\right) \quad ; \quad \lambda_D^{-2} = \frac{1}{\epsilon_0} \sum_\alpha \frac{n_{0\alpha} q_\alpha^2}{k_B T_\alpha}$$

Debye length:

$$\lambda_D \propto \sqrt{\frac{T}{n}}$$

Plasma parameter:

$$\Lambda = n_0 \lambda_D^3 \gg 1$$

Number of particles in a Debye sphere:

$$N = \frac{4\pi}{3} n_0 \lambda_D^3$$

"Definition of plasma"

$$\frac{1}{\sqrt[3]{n_0}} \ll \lambda_D \ll L$$

$L$  is the size of the system

# Collisions

Cross section:  $\sigma$  (m<sup>2</sup>)      Mean free path:  $l_{mfp} = 1/(n\sigma)$

Collision frequency:  $\nu_c = n\sigma v$

Hannu Koskinen Univ of Helsinki

$n$  = density of atoms (and ions)

Total collision cross section:

$$\sigma_{\text{total}} = \sigma_{\text{excitation}} + \sigma_{\text{ion}} + \sigma_{\text{attachment}} + \sigma_{\text{other}}$$

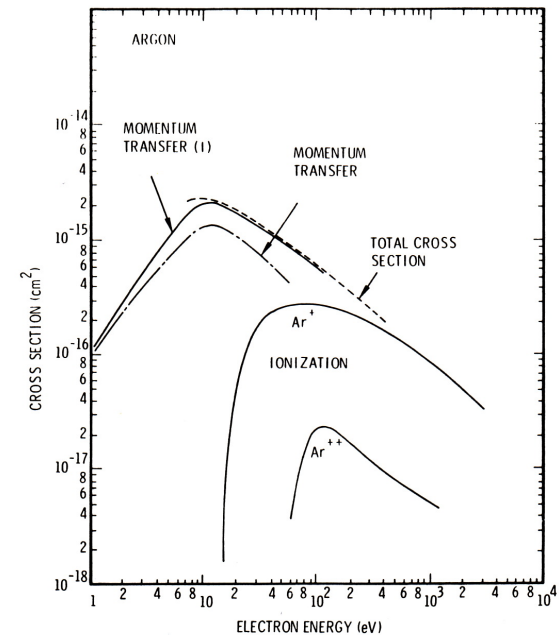
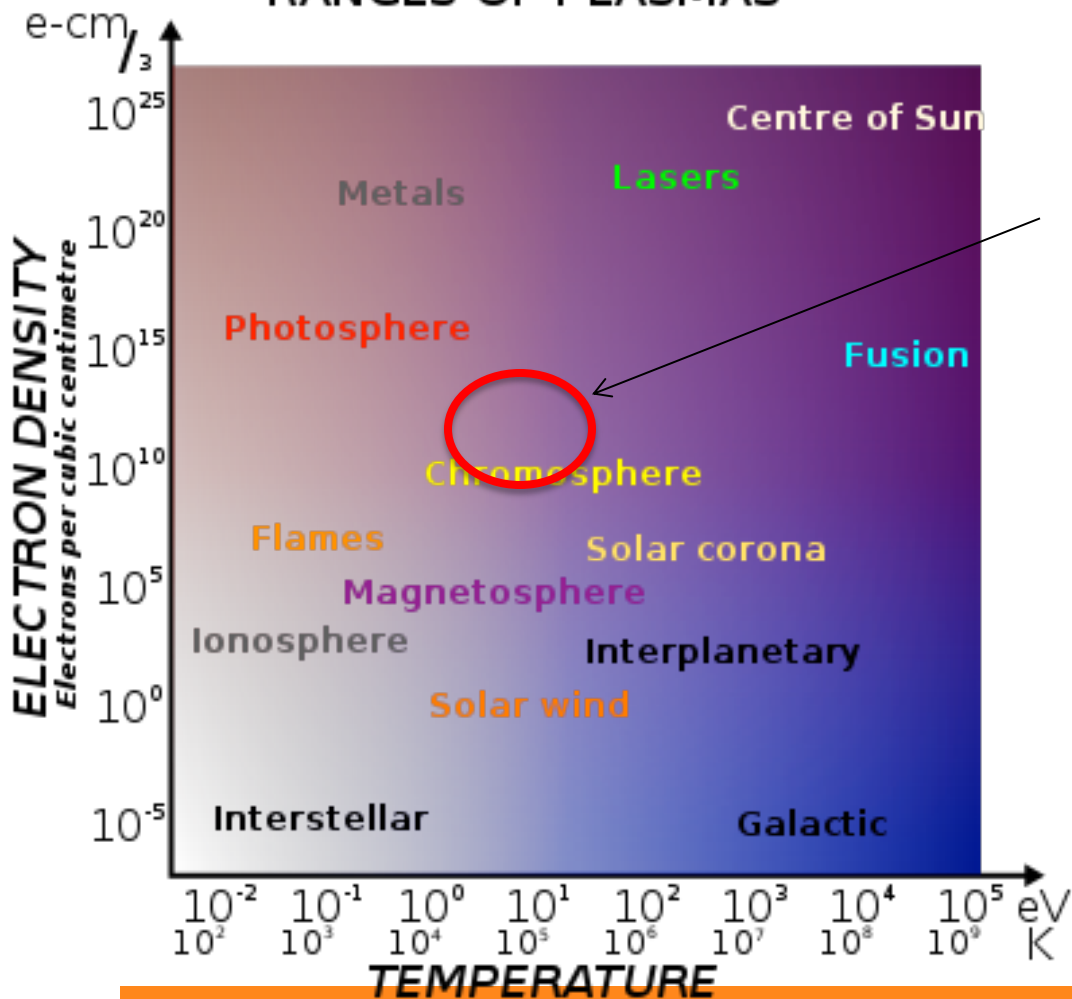


Figure 2.1. Collision cross sections for electrons in Ar gas (from Ref. 1).

Bunshah, Handbook of Deposition Technologies for Films and Coatings Noyes

# Different types of plasmas

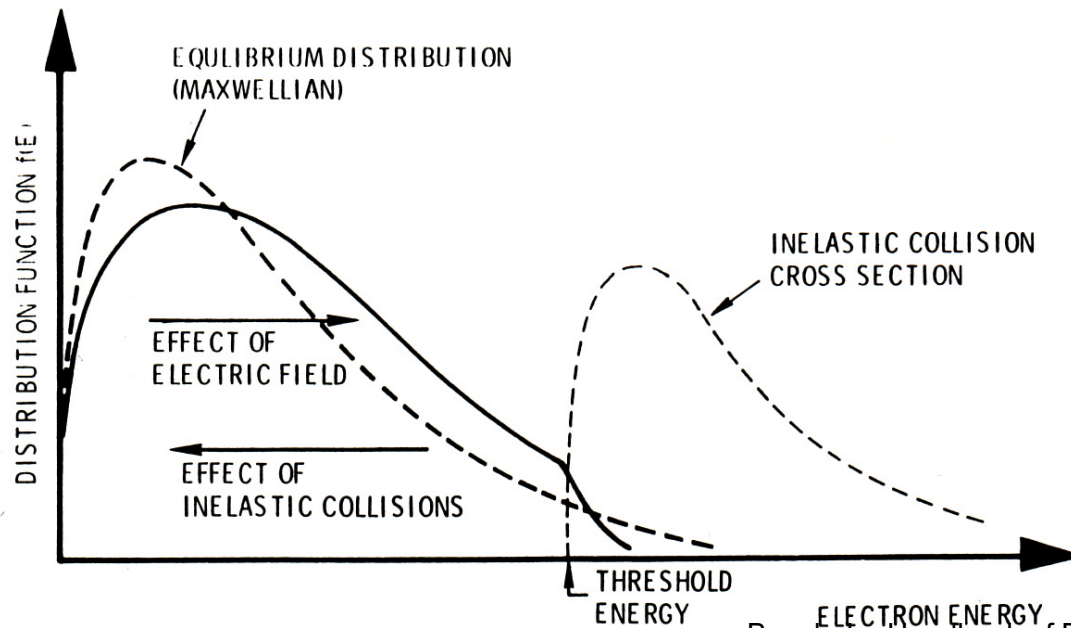
## RANGES OF PLASMAS



Thin film plasma processes

Wikipedia

# Electron temperature



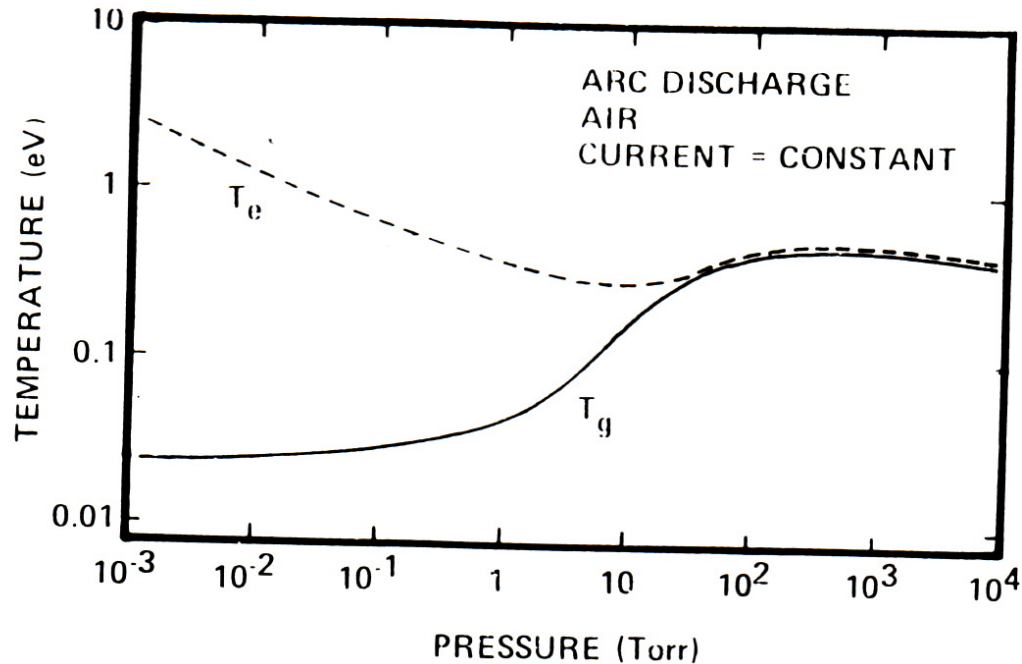
Bunshah, Handbook of Deposition Technologies for  
Films and Coatings Noyes

**Figure 2.4.** Schematic illustration of electron energy distribution function and inelastic collision cross section.

A



# Electron and ion temperature



**Figure 2.3.** Electron ( $T_e$ ) and gas temperatures ( $T_g$ ) in an air arc as a function of pressure (from Ref. 5).

Bunshah, Handbook of Deposition Technologies for Films and Coatings Noyes

# Plasma sheath

Sheath thickness  $d_s \sim \text{constant} * \lambda_D$   
 constant  $\approx 5 - 40$

Glow discharge  $d_s \approx 0.15 - 2 \text{ mm}$

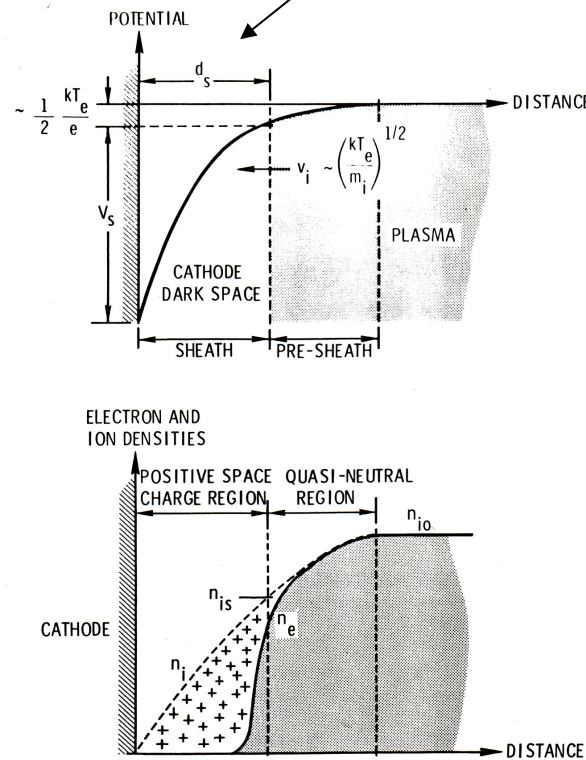
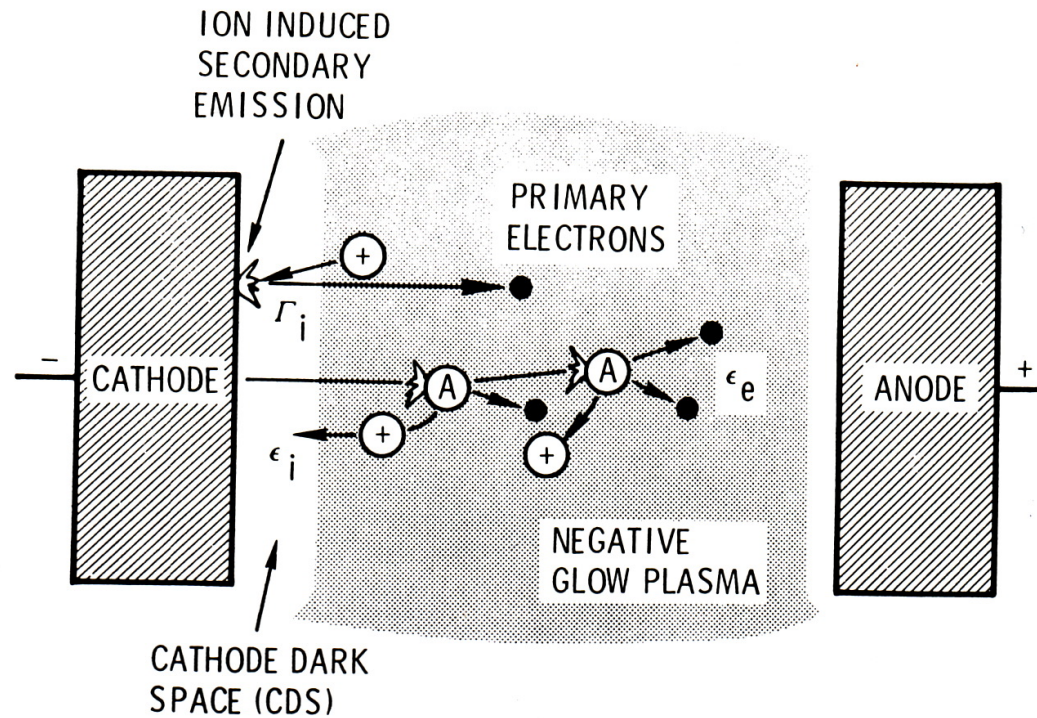


Figure 2.9. Schematic representation of the positive space-charge sheath that develops over a cathode (from Ref. 1).

Bunshah, Handbook of Deposition Technologies for Films and Coatings Noyes

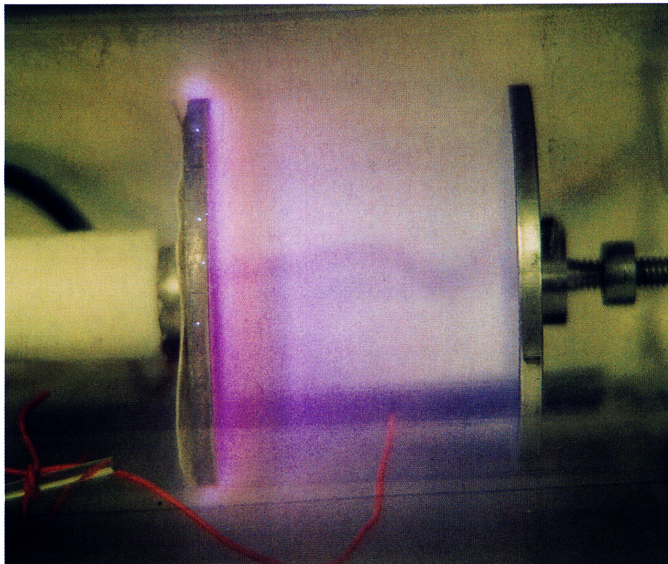
# Cold cathode discharge



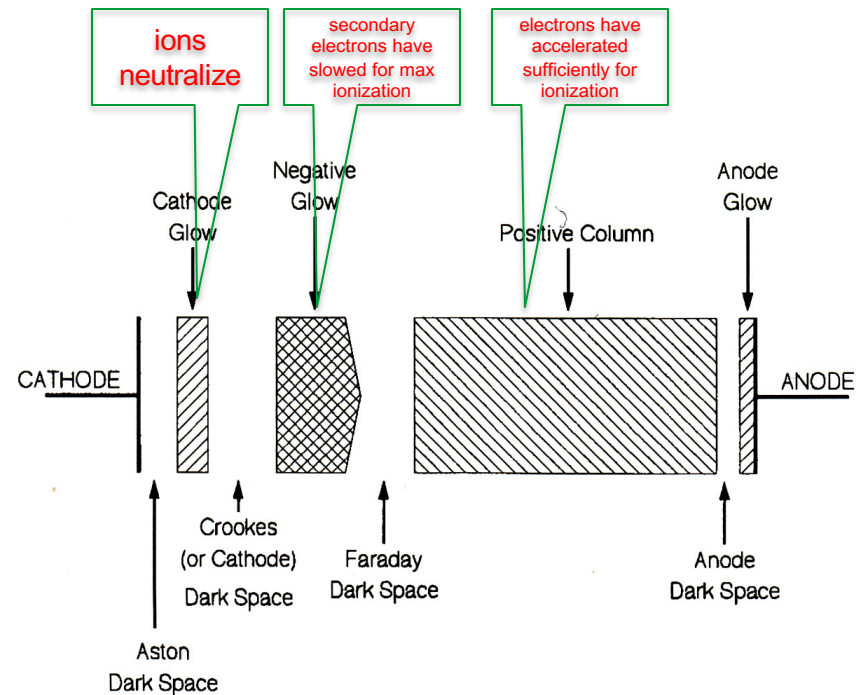
**Figure 2.18.** Schematic illustration of a cold-cathode discharge.

Bunshah, Handbook of Deposition Technologies for Films and Coatings Noyes

# Luminous regions in DC plasma



**Colorplate VI.18** A DC glow discharge in argon. The anode (grounded) is on the right and the cathode (supported by a white teflon insulator) on the left. The orange wire is a Langmuir probe whose bare tip enters the positive column of the discharge. The positive column is the largest luminous region, which extends about 75% of the way from the anode toward the cathode. The pressure was 100 mtorr and the voltage applied between cathode and anode was 1 kV. The discharge current density was 0.22 mA/cm<sup>2</sup>.



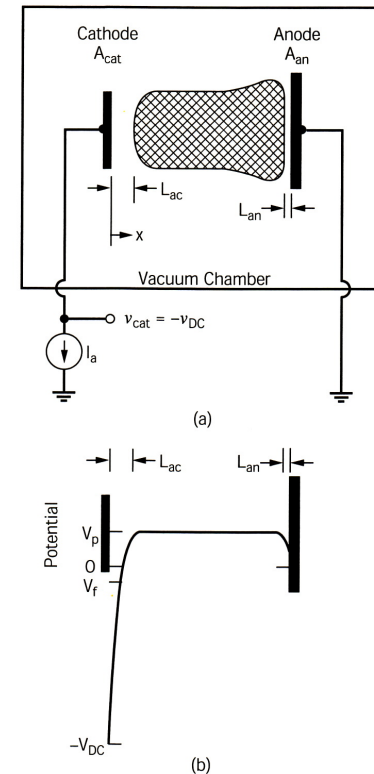
**Figure VI.17** The classical luminous and dark regions of a DC glow discharge, based on classifications by early researchers [Holland, 1956; Maissel and Glang, 1970; Brown, 1966; Nasser, 1971; Llewellyn-Jones, 1966; Cobine, 1941; von Engel, 1965].

# Practical sputtering plasma -1

- Argon pressure 1 torr
- atom density ( $n$ )  $3 \times 10^{16} \text{ cm}^{-3}$
- $n_i = n_e$   $10^{10} \text{ cm}^{-3}$
- ionization fraction  $3 \times 10^{-7}$  (weakly ionized plasma)
- ion temperature  $T_i$  300K
- electron temperature  $T_e$  23,000K

# Practical sputtering plasma -2

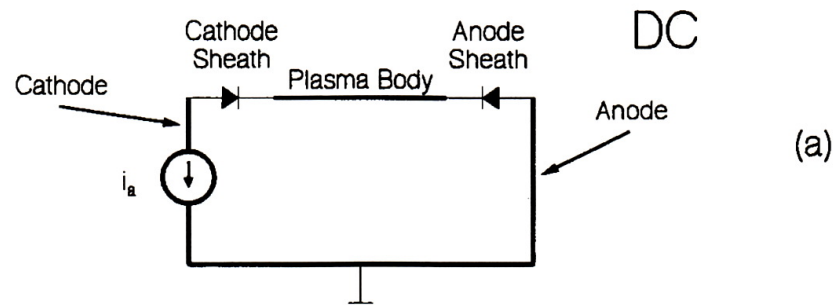
- VDC 1000V
- $V_p$  8V
- Current density at cathode 2 mA/cm<sup>2</sup>
- Cathode sheath  $L$  2 mm
- mean free path  $\lambda$  50  $\mu$ m



**Figure VI.8** (a) Schematic diagram of a DC sputtering discharge; (b) the potential profile (not to scale, as  $V_p - V_f$  is typically much less than  $V_{DC}$ ).



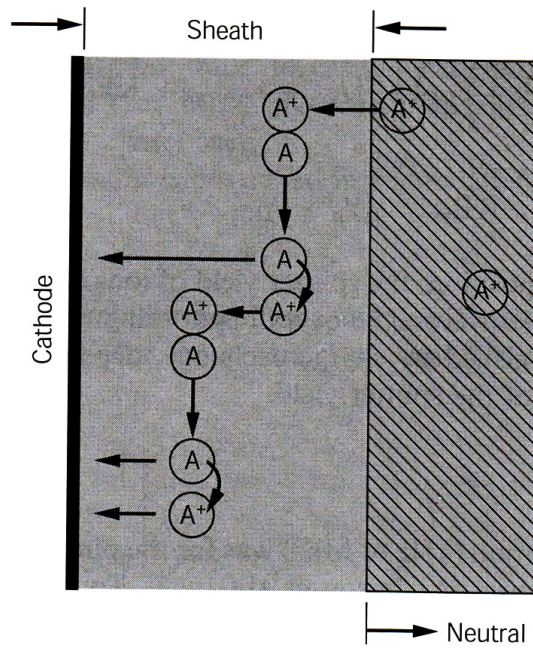
# Circuit models of DC plasma discharge



**Figure VI.9** Circuit models for (a) a DC sputtering discharge and (b) a capacitive RF sputtering discharge.

Mahan, Physical Vapor Deposition of Thin Films, Wiley

# Ion energy at cathode



$$\sigma = 2.5 \times 10^{-15} \text{ cm}^{-3}$$

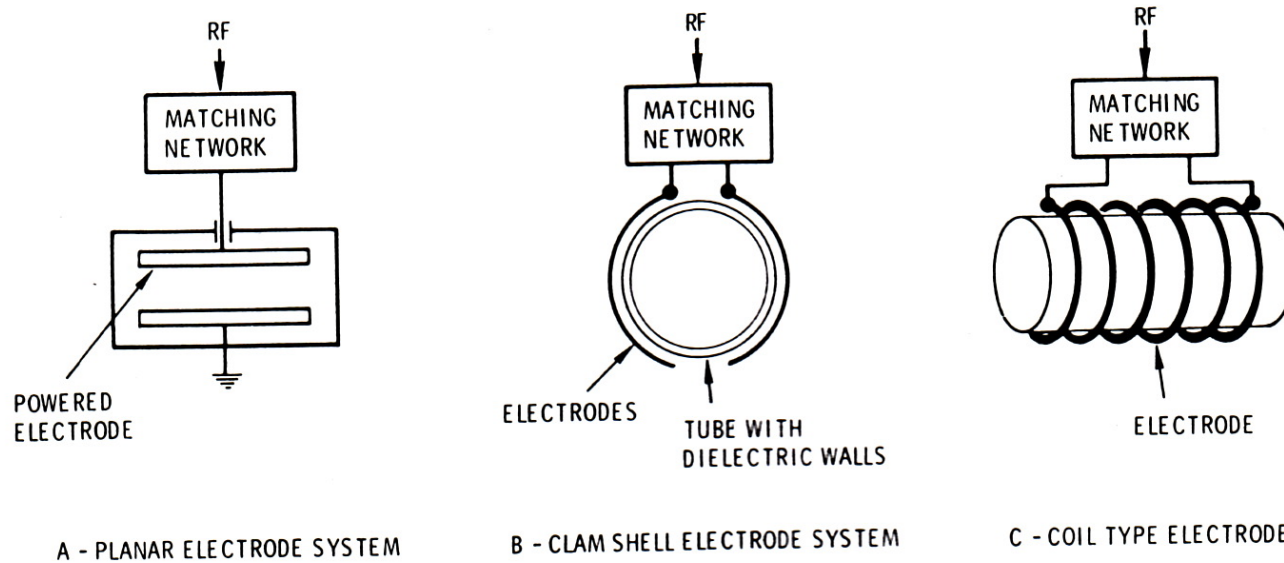
**Figure VI.10** The process of symmetric charge exchange within the cathode sheath. When two charge exchange events occur, as shown here, a single ion entering the sheath is converted into two neutrals plus an ion, all of which strike the cathode (but with kinetic energies corresponding to only a fraction of the cathode fall).

Mahan, Physical Vapor Deposition of Thin Films, Wiley



# AC plasma methods

# AC plasma



**Figure 2.12.** Schematic illustration of glow discharge devices commonly used in plasma-assisted materials processing.

# Forming of self-bias in AC discharge

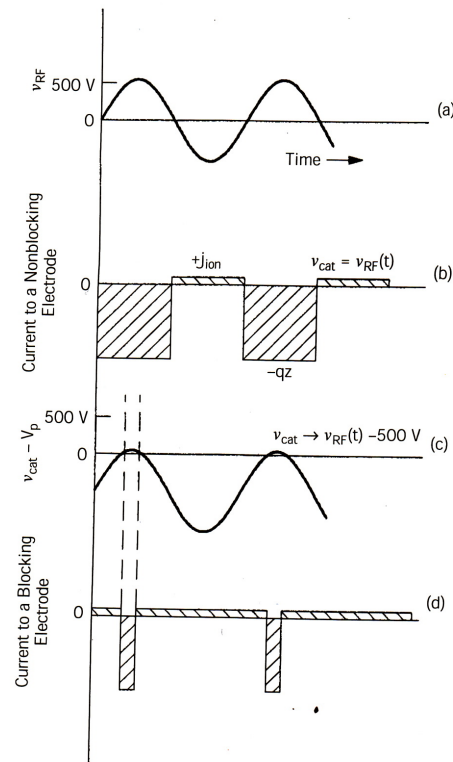


Figure VI.11 DC self-bias. Potentials and currents for RF excitation of (a-b) nonblocking and (c-d) blocking electrodes.

Mahan, Physical Vapor Deposition of Thin Films, Wiley

# Self bias at electrodes

$$\frac{V_1}{V_2} = \left( \frac{A_2}{A_1} \right)^n$$

$n = 4$  (sometimes 2)

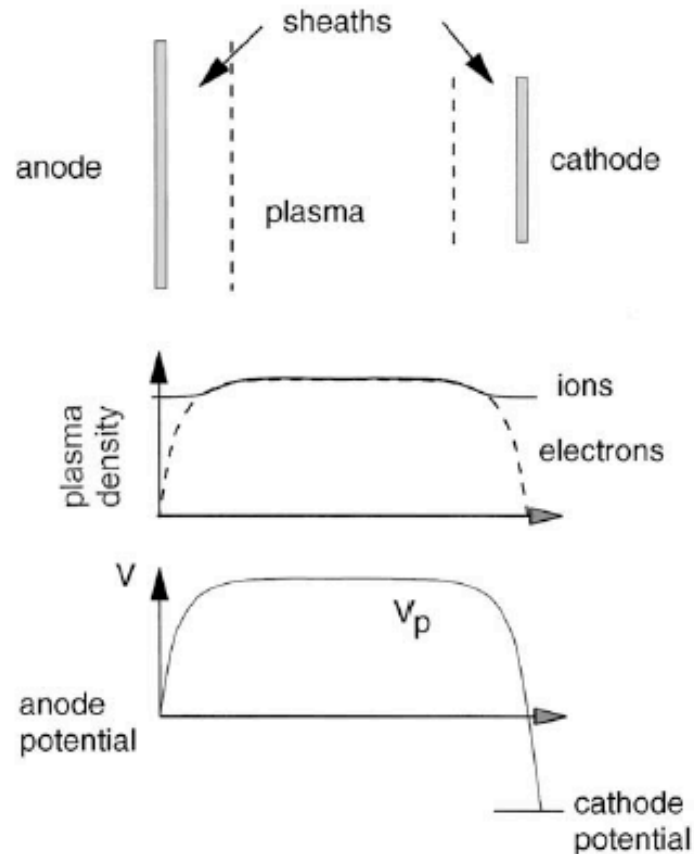
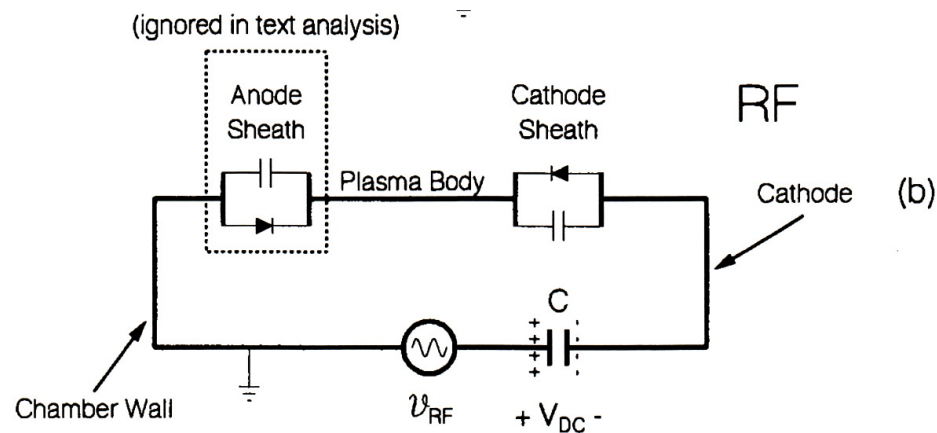


Fig. 7. Electron and ion distributions which create sheaths between the neutral plasma and the walls.

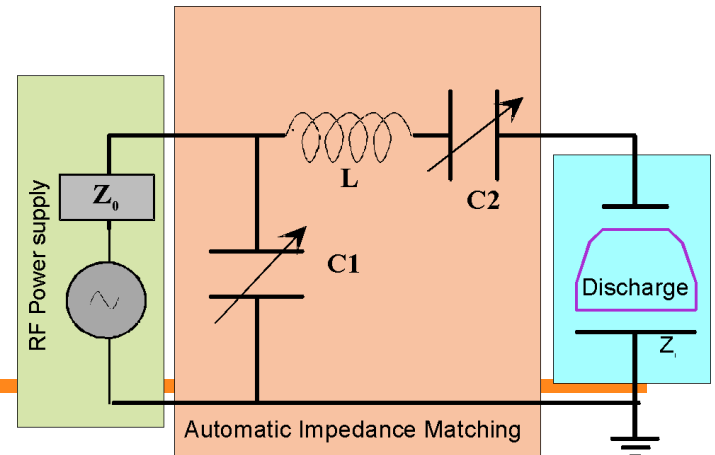
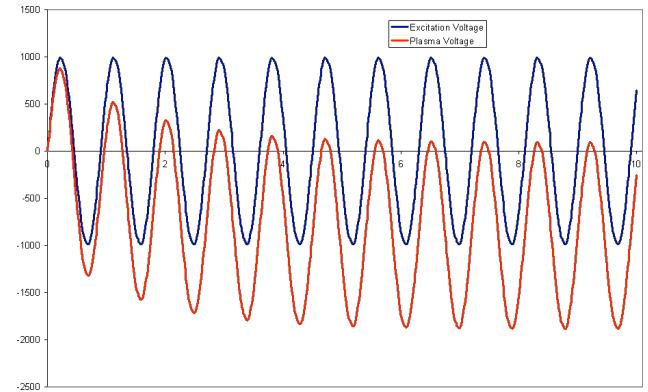
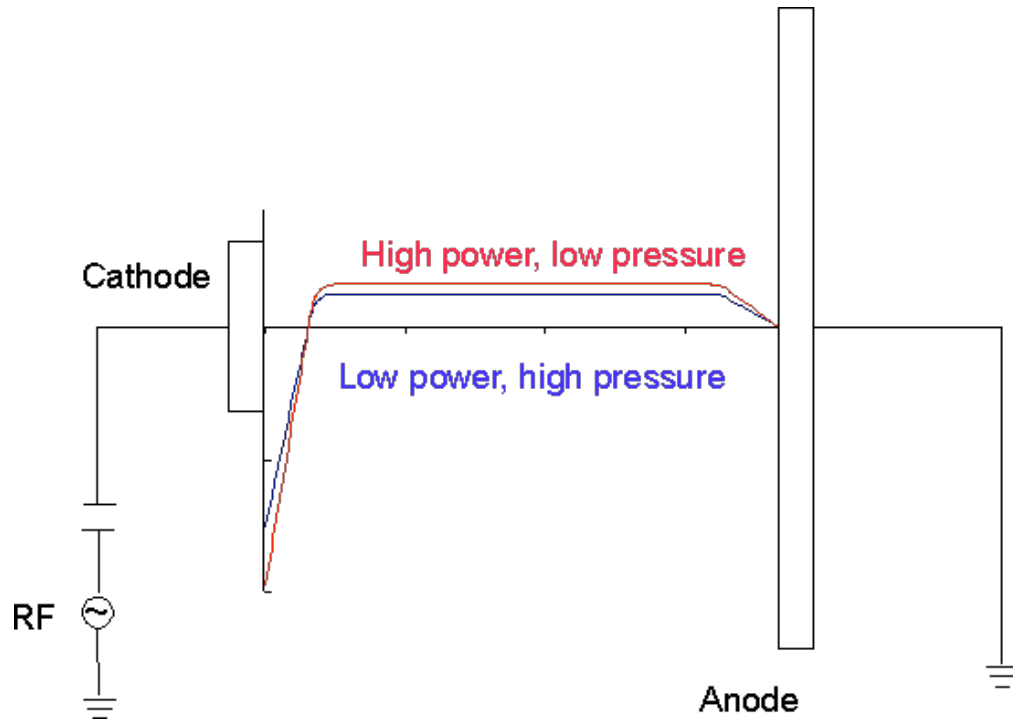
# Circuit models of RF plasma discharge



**Figure VI.9** Circuit models for (a) a DC sputtering discharge and (b) a capacitive RF sputtering discharge.

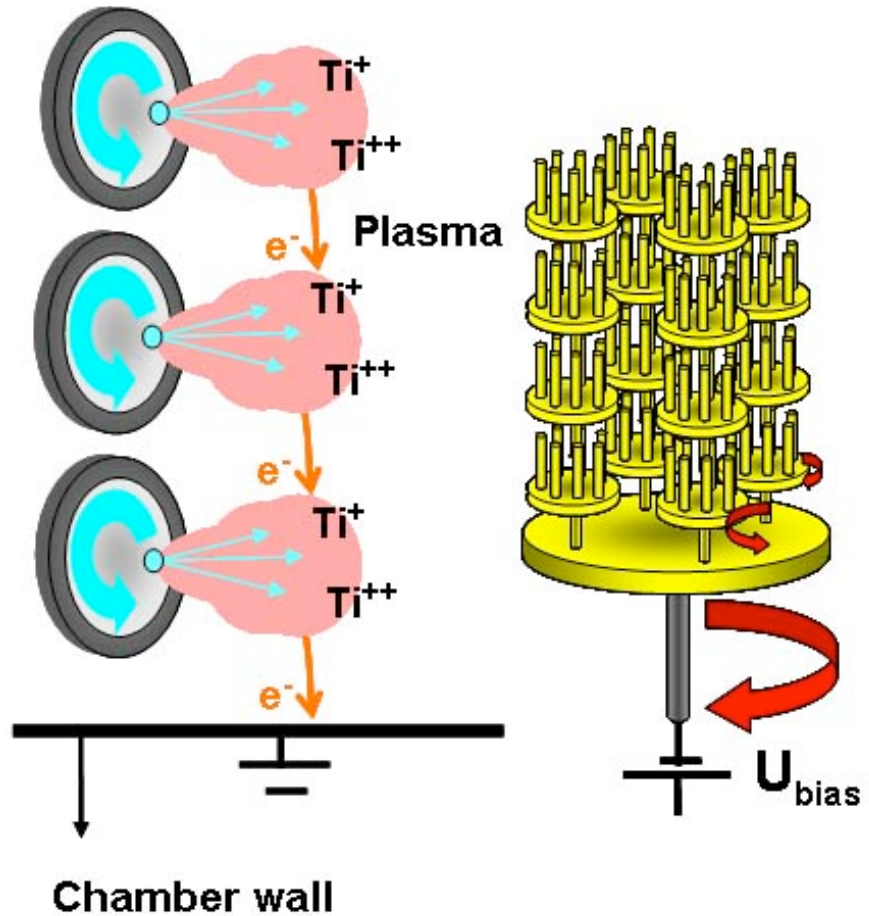
Mahan, Physical Vapor Deposition of Thin Films, Wiley

# RF Plasma glow discharge



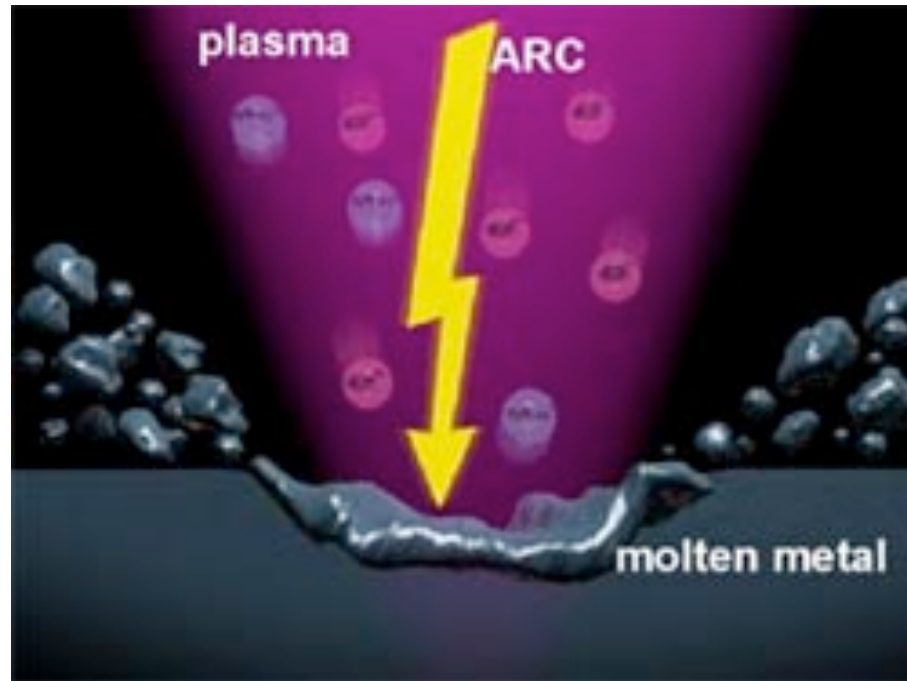
# Arc plasma

# Arc discharge deposition





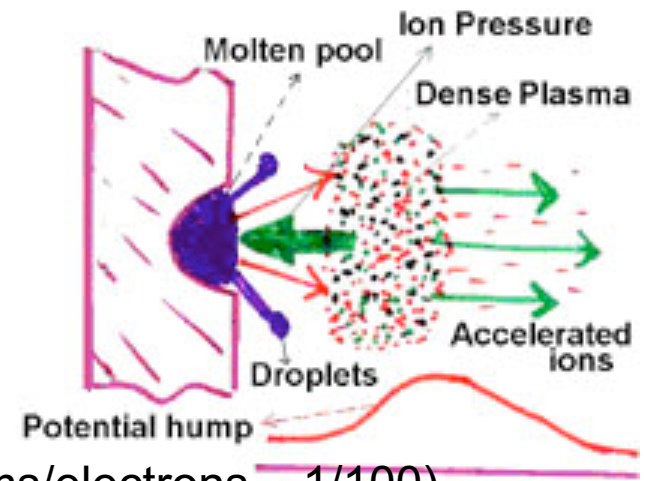
# Arc discharge – cathode spot



[www.shm-cz.cz/files/schema01.jpg](http://www.shm-cz.cz/files/schema01.jpg)

# Arc discharge process

- arc current concentrated into filaments – arcs
- intense electron emission
- intense ion emission due to electron current ( atoms/electrons – 1/100)
- ionization of atoms – formation of plasma
- flow of ions to cathode – intense sputtering of atoms
- $10^6 - 10^8 \text{ A/m}^2$
- overlapping thermal spikes
- materials is melted and sublimated in cathode spots
- cathode spots move randomly or could be steered by using magnets
- electrons ionize vapor and create more electrons – increase of current
- ions accelerate
  - due to potential difference in plasma
  - due to multiple collisions with fast electrons
- macro particles (up to  $10 \mu\text{m}$  diam.) are formed



Timko, Nordlund  
simulations

<http://prb.aps.org/supplemental/PRB/v81/i18/e184109>

## Filtered arc

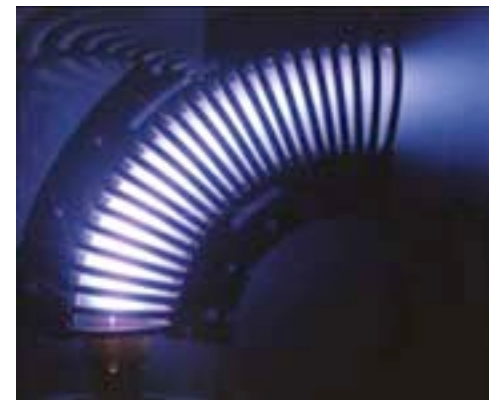
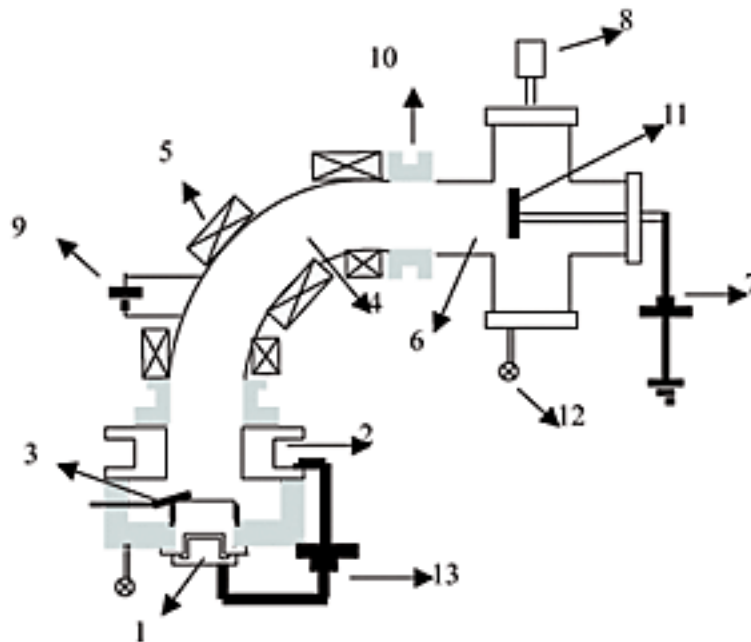
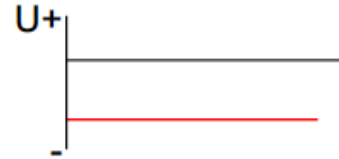


Figure 1. Scheme of the DCF2 device. (1) cathode; (2) anode; (3) trigger; (4) quarter torus magnetic filter; (5) torus coil; (6) deposition chamber; (7) probe bias source; (8) diagnostic port; (9) filter bias source; (10) insulators; (11) collecting probe; (12) vacuum pumping systems; (13) arc source.

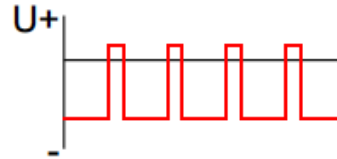
# PULSED SPUTTERING

## Definitions

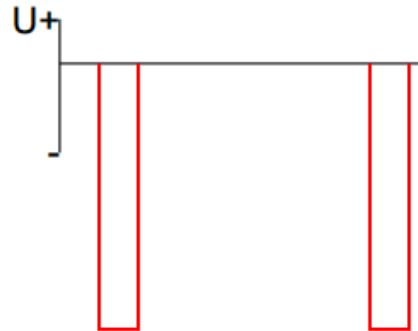
- DC-sputtering



- Pulsed DC



- HiPIMS



# HIPIMS

# High Power Pulsed Magnetron Sputtering (HIPIMS)

- Introduced by Kouznetsov et al.\*
  - Also known as HIPIMS – High Power Impulse Magnetron Sputtering
- High power pulses of short duration
  - Peak value typically 100 times greater than conventional magnetron sputtering
    - Peak power densities of 1-3 kW/cm<sup>2</sup>
  - Pulse width of 100 - 150 μsec
  - Discharge voltages of 500-1000 V

\*V. Kouznetsov, K. Macák, J. M. Schneider, U. Helmersson, and I. Petrov, "A New Sputter Technique Utilizing Very High Target Power Densities," Surf. Coat. Tec

RSI W. Sproul, AEPSE 2009 Tutorial    The Practice of Reactive Sputter Deposition



Pulsed Plasma  
Diffusion™

# HIPIMS

- **High degree of target material ionization**
  - High secondary electron current
    - Promotes ionization of sputtered species
  - Can approach 100%, vs. up to ~10% for conventional sputtering
- **Potential is to use the ions to improve film properties and structure of coatings**
  - With bias can produce dense films and coat irregular shapes
  - With high ion flux and low bias voltage should be possible to deposit low stress thick films

## Loss of Deposition Rate\*

Power, kW	Al Rate, nm min <sup>-1</sup>		Ratio, HPPMS to DC
	HPPMS	Pulsed DC	
1.0	22	70	0.31
2.0	37	149	0.25

- **HIPIMS** rate loss partially due to ionized sputtered species being attracted back to the target

\*W. D. Sproul, D. J. Christie, and D. C. Carter, "The Reactive Sputter Deposition of Aluminum Oxide Coatings Using High Power Pulsed Magnetron Sputtering (HPPMS)," Society of Vacuum Coaters, 47<sup>th</sup> Annual Technical Conference Proceedings (April 24-29, 2004) Dallas, TX, pp. 96-100.



# Fluxes of ions in HIPIMS

786

André Anders J. Vac. Sci. Technol. A, Vol. 28, No. 4, Jul/Aug 2010

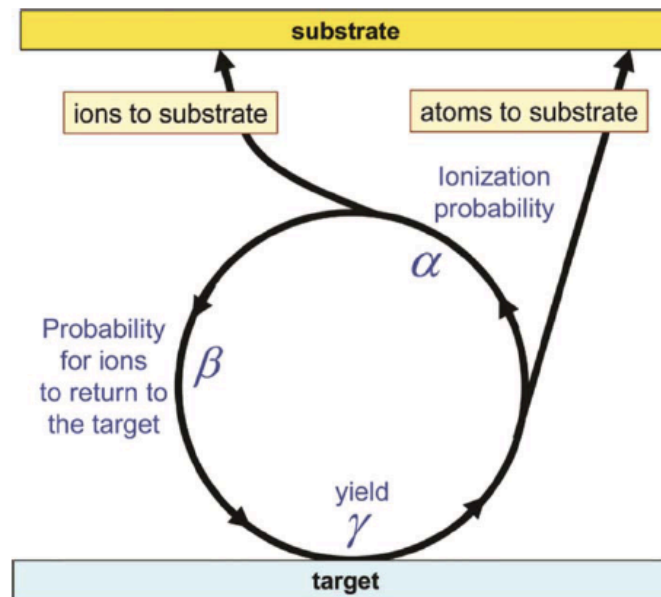


FIG. 2. (Color online) Schematic presentation of the fluxes involved in the deposition by HIPIMS under conditions when the plasma is dominated by metal sputtered from the target;  $\alpha$ ,  $\beta$ , and  $\gamma$  are the ionization probability, the return probability, and the sputtering yield, respectively; for further explanations see text.

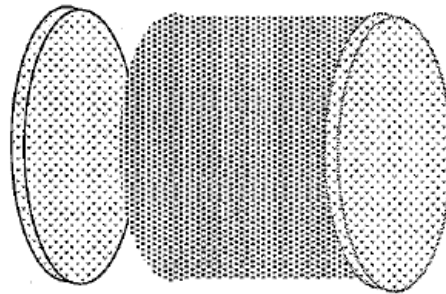
# Reactive sputtering

## Reactive Sputtering

- **Sputtering of an elemental target in the presence of a gas (in addition to the inert gas) that will react with the element to form a compound**
  - **Examples:**
    - $\text{Al} + \text{O}_2$  to form  $\text{Al}_2\text{O}_3$
    - $\text{Ti} + \text{N}_2$  to form  $\text{TiN}$
- **Purposely add the reactive gas**
- **Outgassing can be a factor**

# Reactive sputtering

## Reactive Sputtering



**Target + Reactive gas = Film**

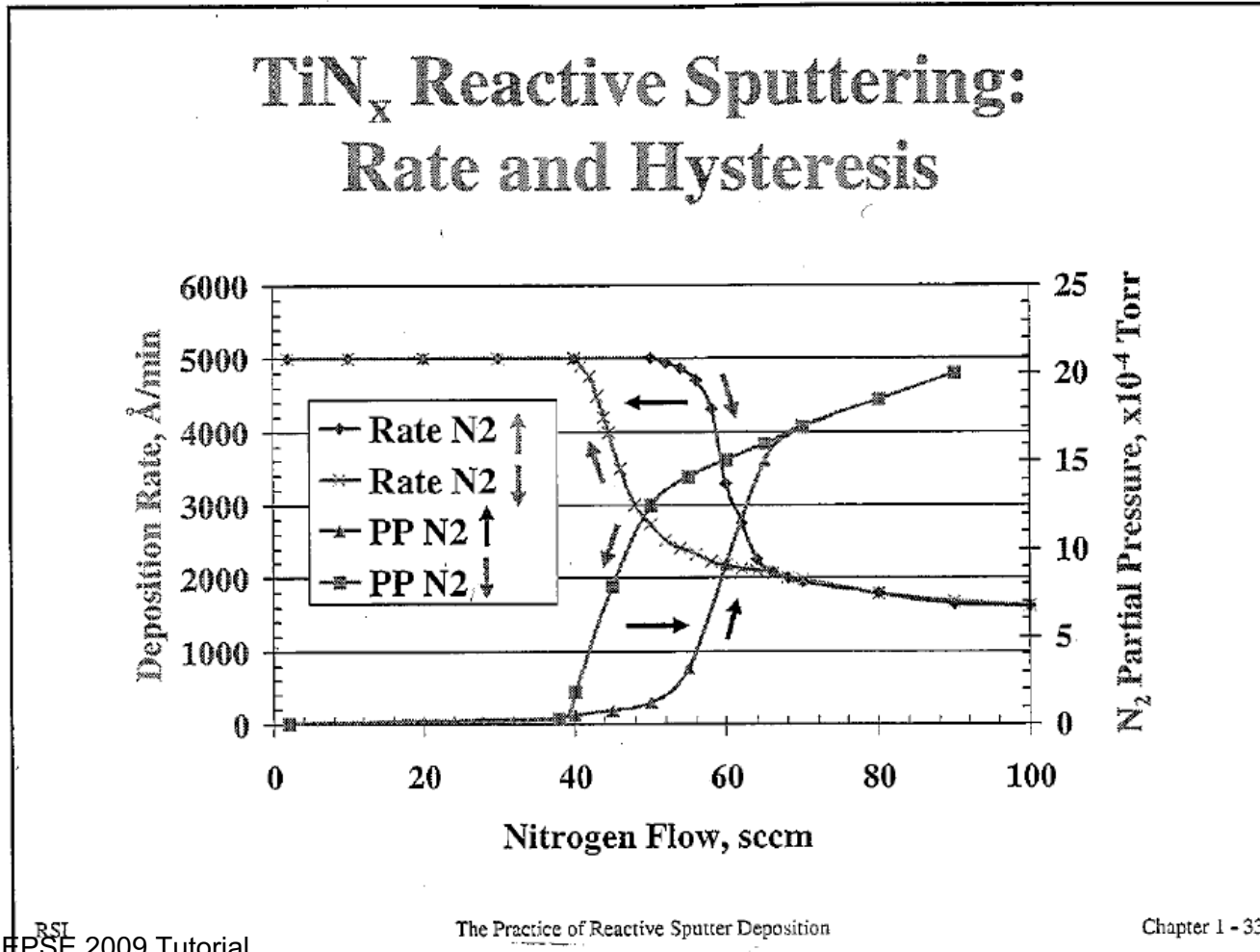
1. Doping:  $\text{Ta} + \text{N}_2 = \text{TaN}_x$
2. Compound formation:  $\text{Ta} + \text{O}_2 = \text{Ta}_2\text{O}_5$

# Reactive sputtering

## Metal vs. Poisoned Mode

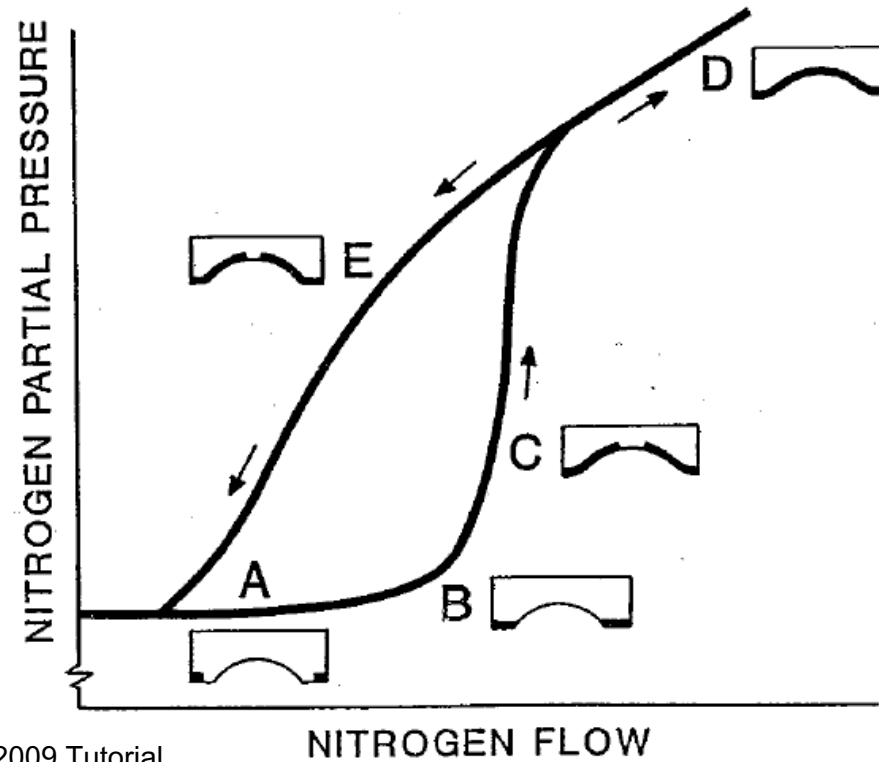
- **Metal mode**
  - Sputtering metal
  - Reactive gas partial pressure low
- **Poisoned mode**
  - Target covered with compound
  - Reactive gas partial pressure high
- **Target can be partially reacted**
  - Takes partial pressure control

# Reactive sputtering



# Reactive sputtering

## Flow Control Hysteresis Loop



W. Sproul, AEPSE 2009 Tutorial

# Reactive sputtering

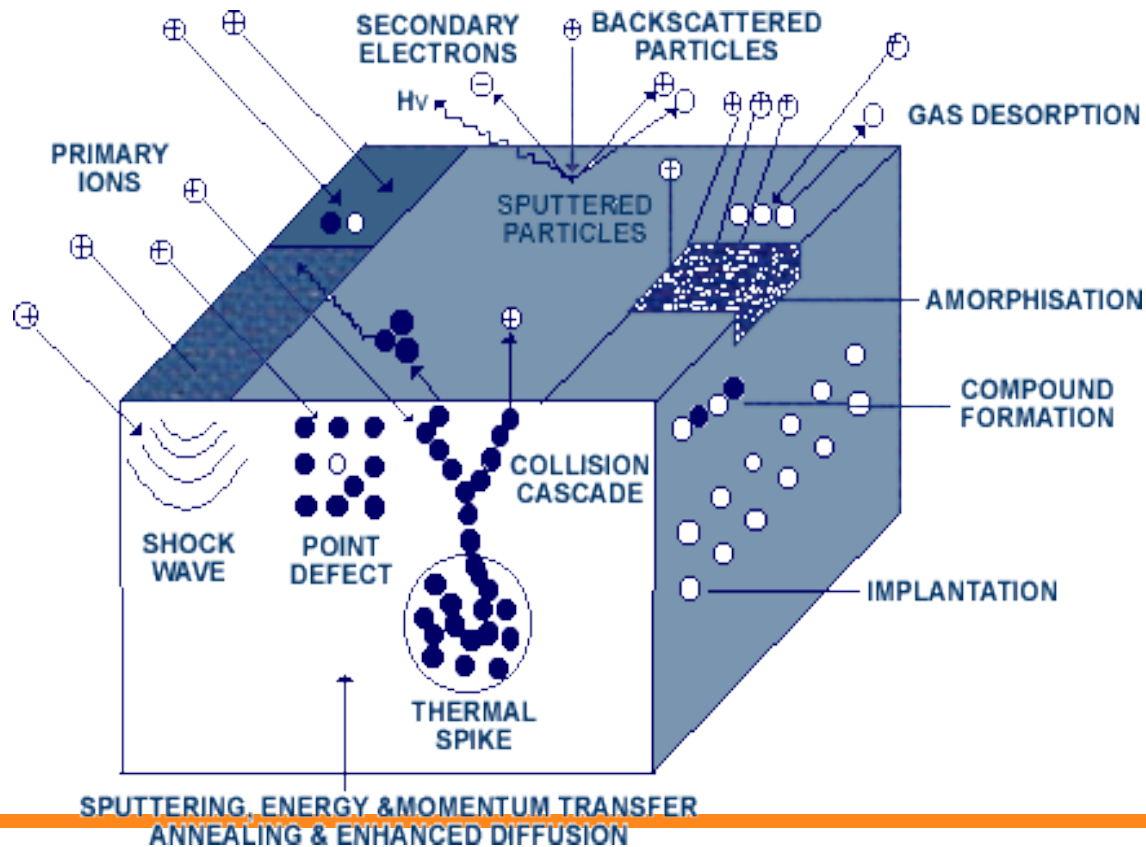
## Reactive Deposition Examples

<u>Target</u>	H <sub>2</sub>	N <sub>2</sub>	O <sub>2</sub>	H <sub>2</sub> S	AsH <sub>3</sub>	Ga(CH <sub>3</sub> )
Al		AlN	Al <sub>2</sub> O <sub>3</sub>			
Ti	TiH	TiN	TiO <sub>2</sub>			
Ta	TaH	Ta <sub>2</sub> N, TaN	Ta <sub>2</sub> O <sub>5</sub>			
Cu			CuO	Cu <sub>2</sub> S		
B		BN				
C		CN				
Si	Si:H	Si <sub>3</sub> N <sub>4</sub>	SiO <sub>2</sub>			
In <sub>9</sub> Sn <sub>1</sub>			ITO			
Zn			ZnO			
Sb						GaSb
LiNbO <sub>3</sub>			LiNbO <sub>3</sub>			
GaAs					GaAs	
ZnO	ZnO <sub>1-x</sub>		ZnO			

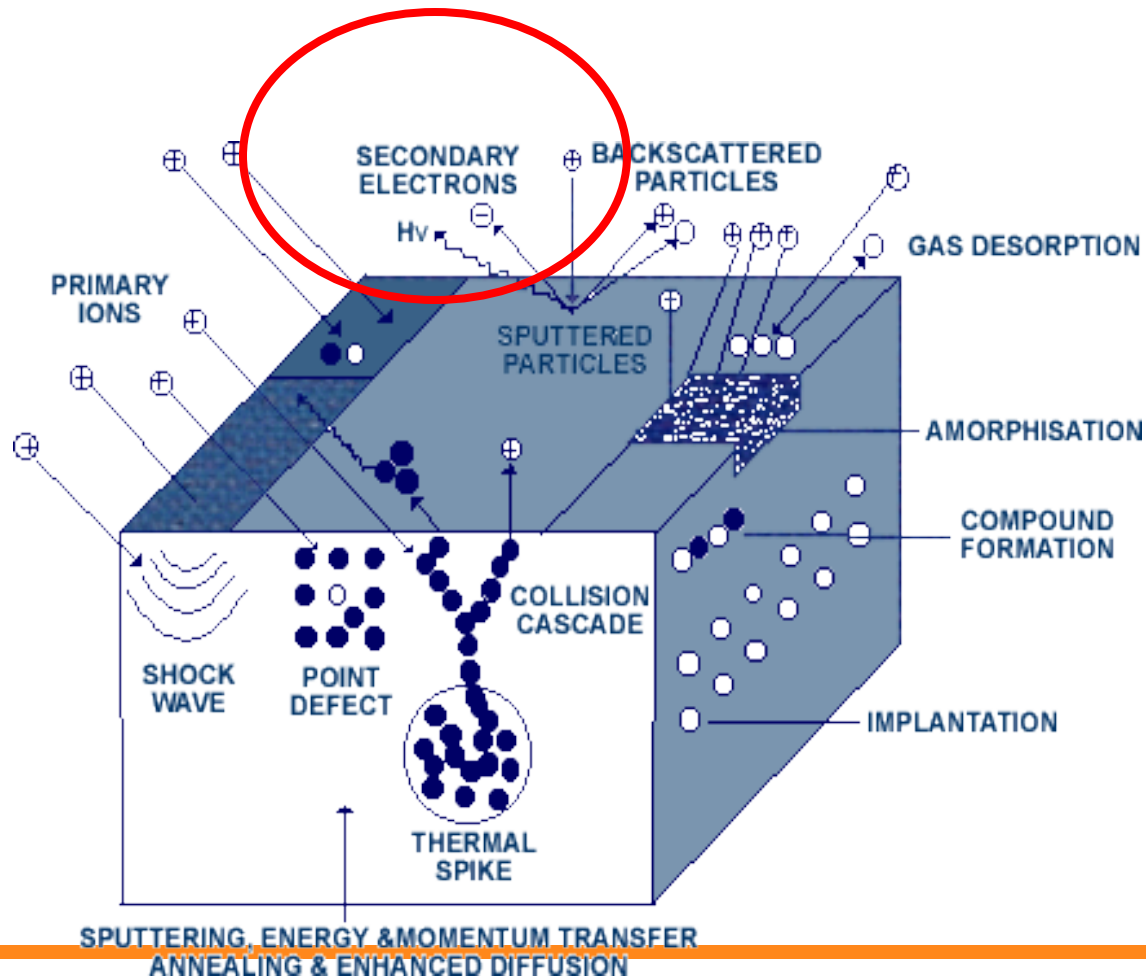
# Ion solid interactions



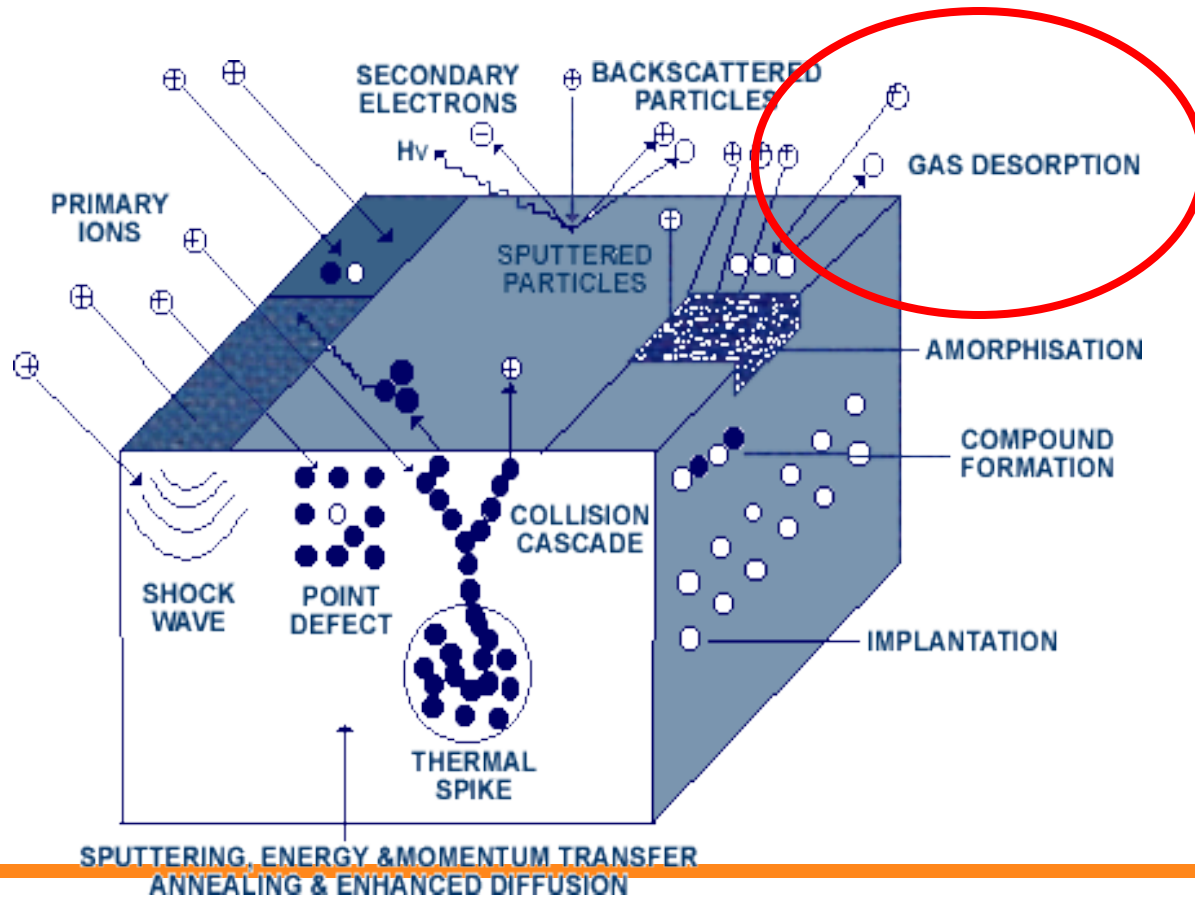
# Energetic ion surface interactions



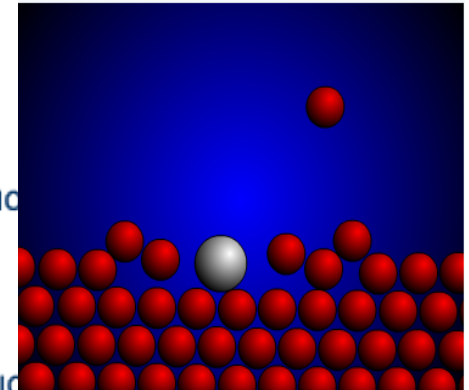
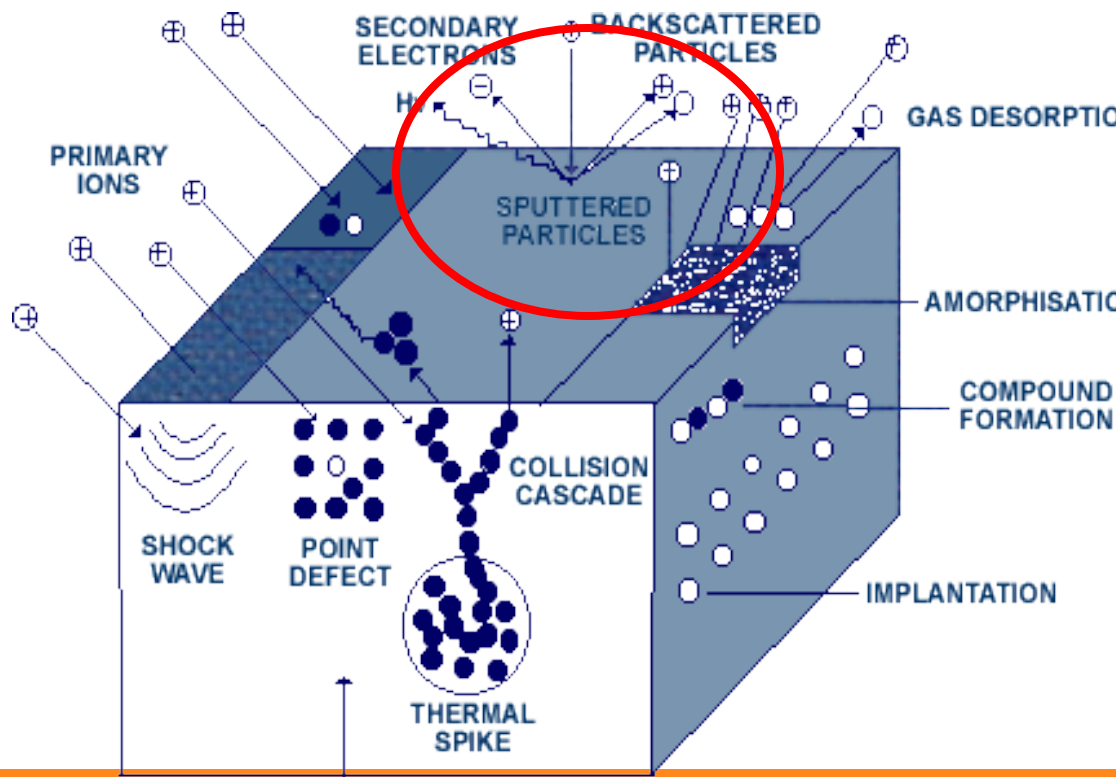
# Secondary electrons



# Desorption, cleaning

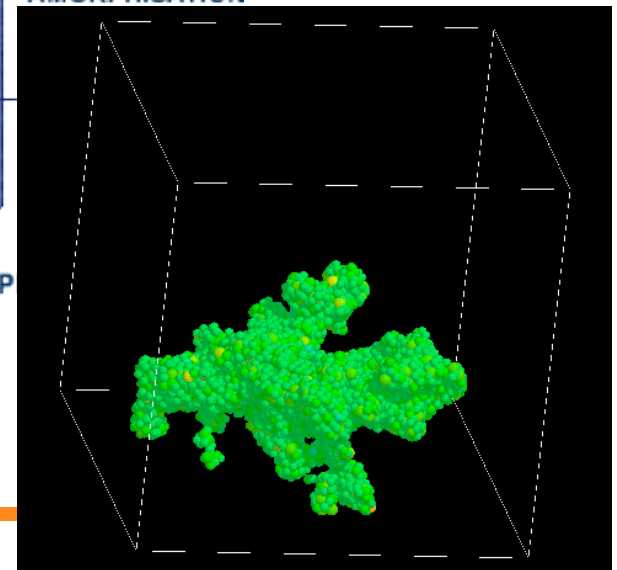
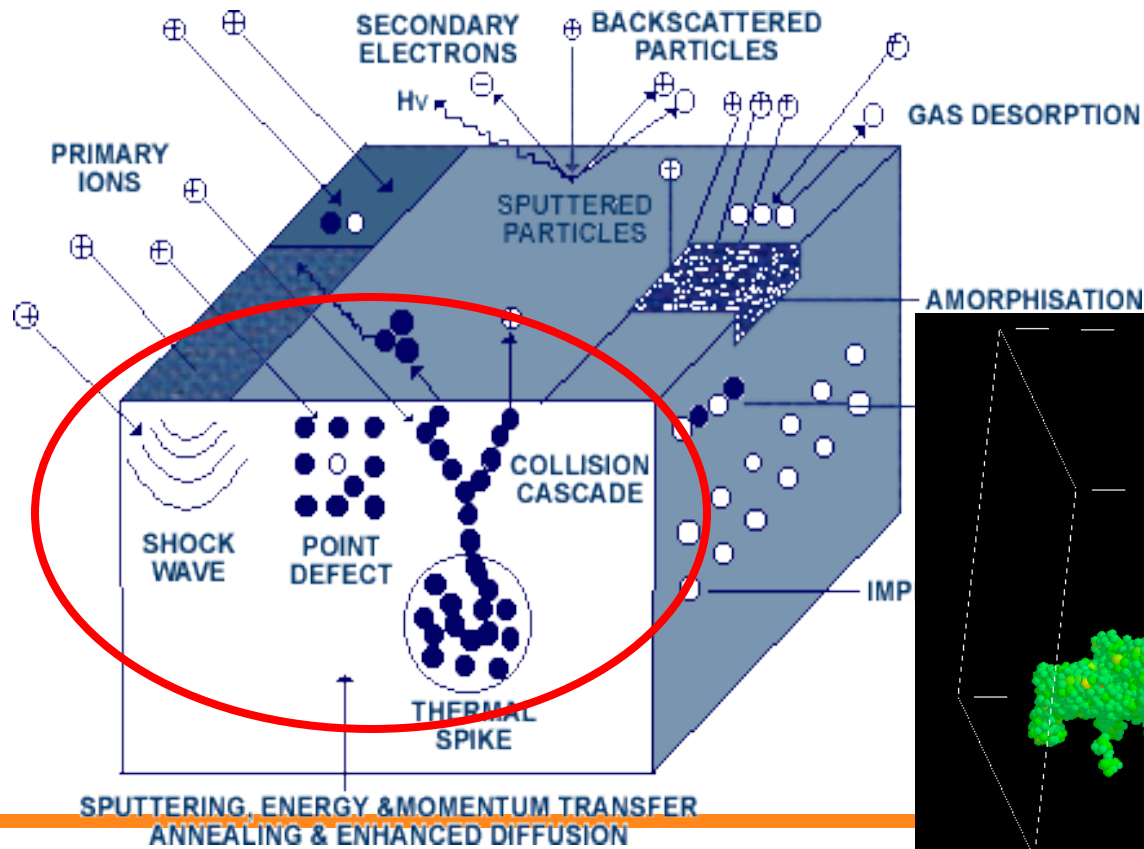


# Sputtering

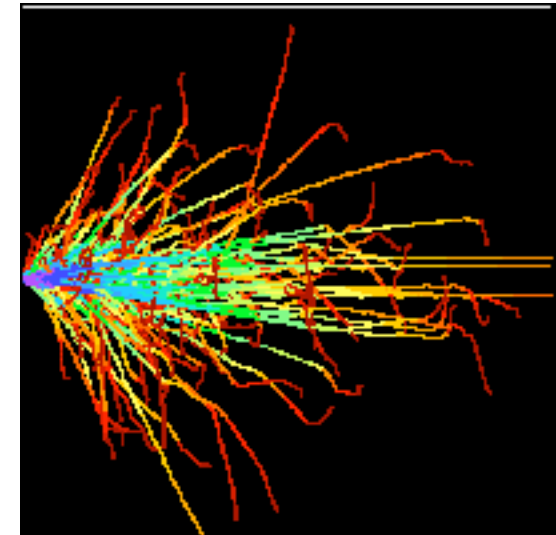
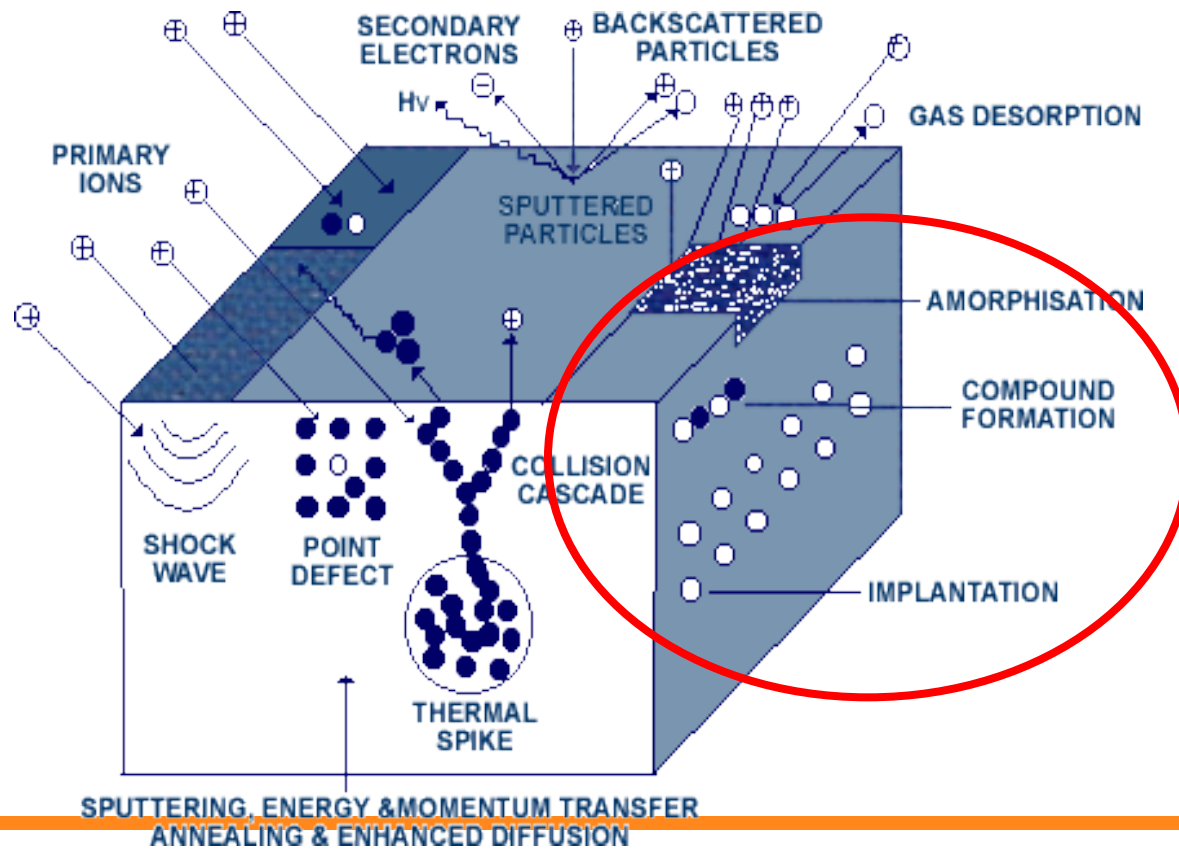


SPUTTERING, ENERGY & MOMENTUM TRANSFER  
ANNEALING & ENHANCED DIFFUSION

# Collision cascade, thermal spike

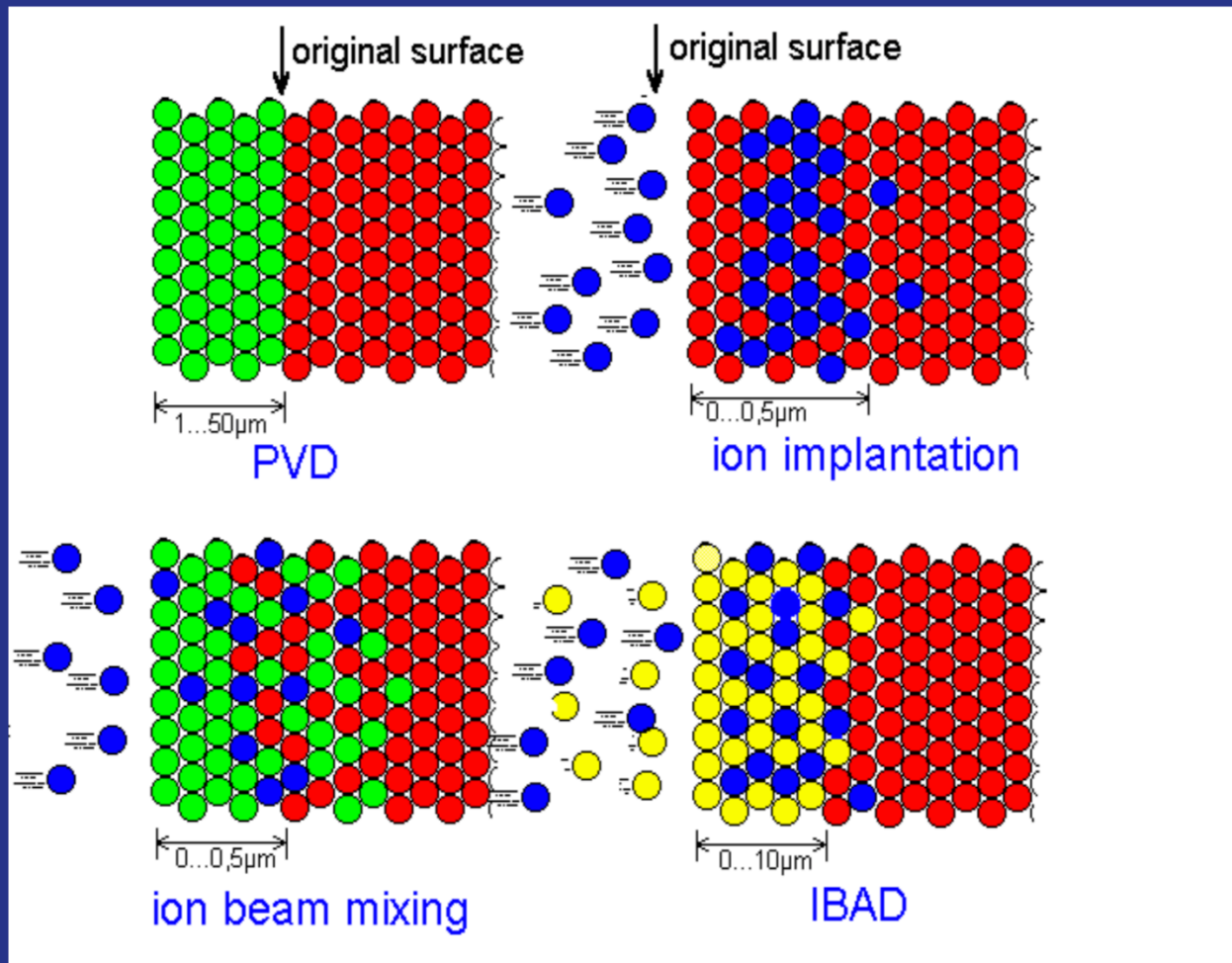


# doping, compounds



# PVD and Ion Assisted Processes

## Which role can energetic ions play



# Sputtering

- Source of atoms and ions
- Cleaning: Removing loose atoms, impurities, oxides



# Sigmund Theory

$$S = \frac{3\alpha 4M_1M_2E}{4\pi^2(M_1 + M_2)^2U_s}$$

Good for low energy (<1keV)

where:

$\alpha$  is a function of  $M(\text{target})/M(\text{ion})$  and  
incident angle  $0.1 > \alpha > 1.4$

but often has a value of 0.2 - 0.4

$M_1$  is the Mass of the ion

$M_2$  is the mass of the target

$E$  is incident ion energy

$U_s$  is the binding energy of the target ions

# Sputtering yield

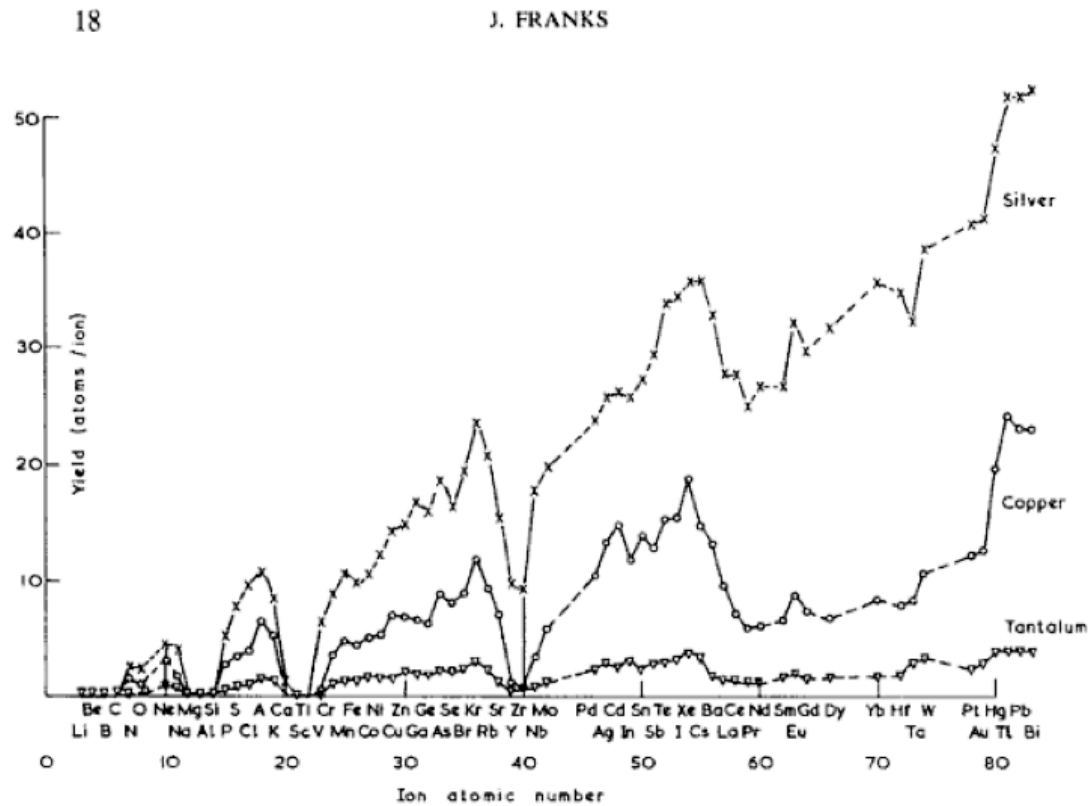
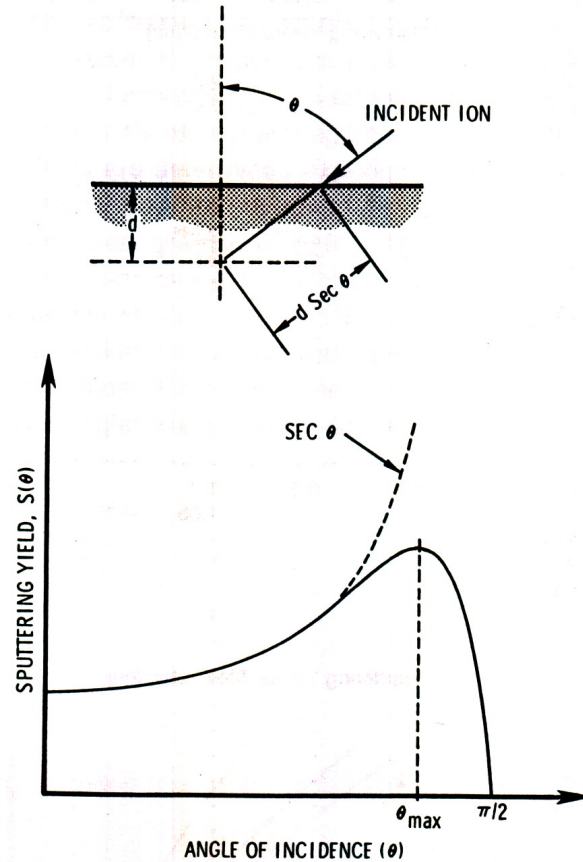
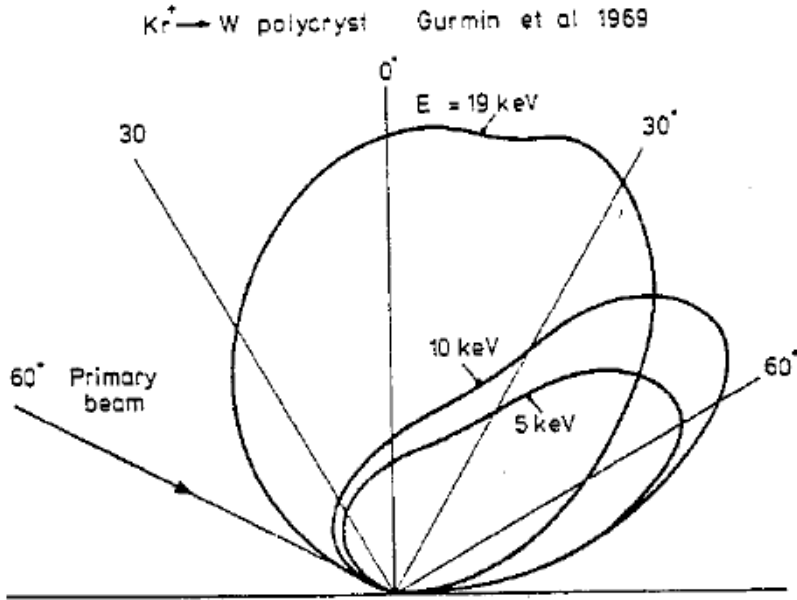


FIG. 15. Sputtering yield of silver, copper, and tantalum as a function of bombarding ion atomic number (Spencer and Schmidt, 1971).

# Sputter yield angle dependence



**Figure 5.7.** Schematic diagram showing variation of the sputtering yield with ion angle of incidence for a constant ion energy.

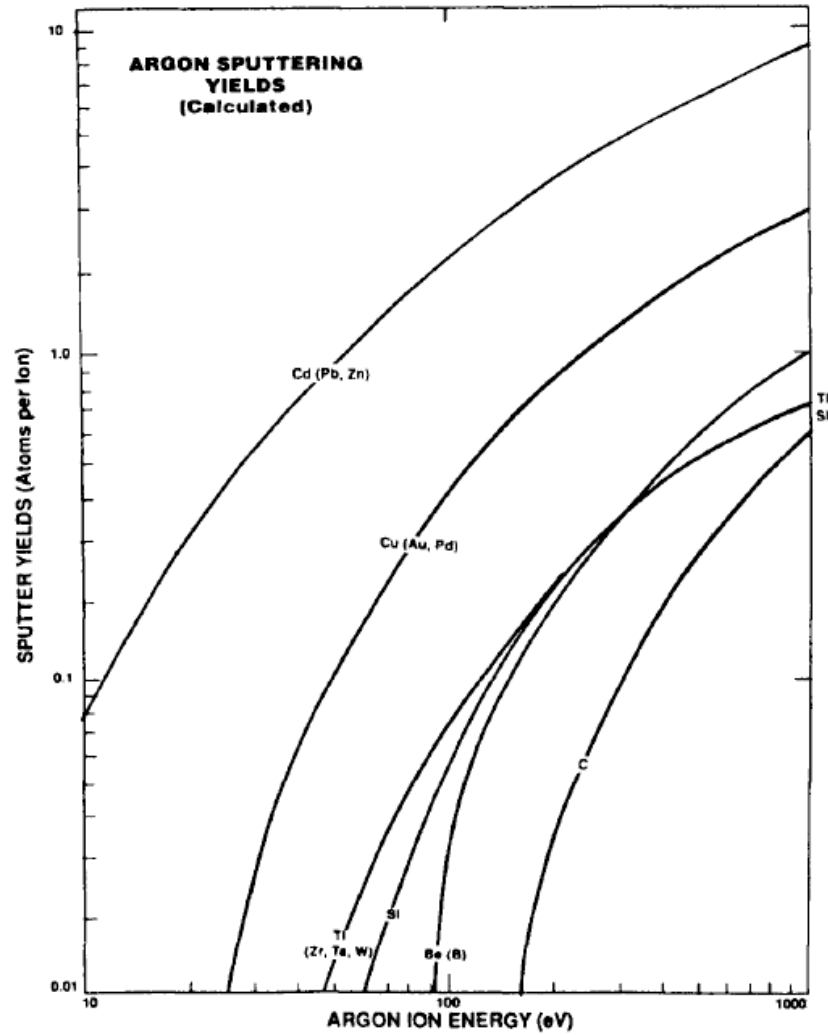
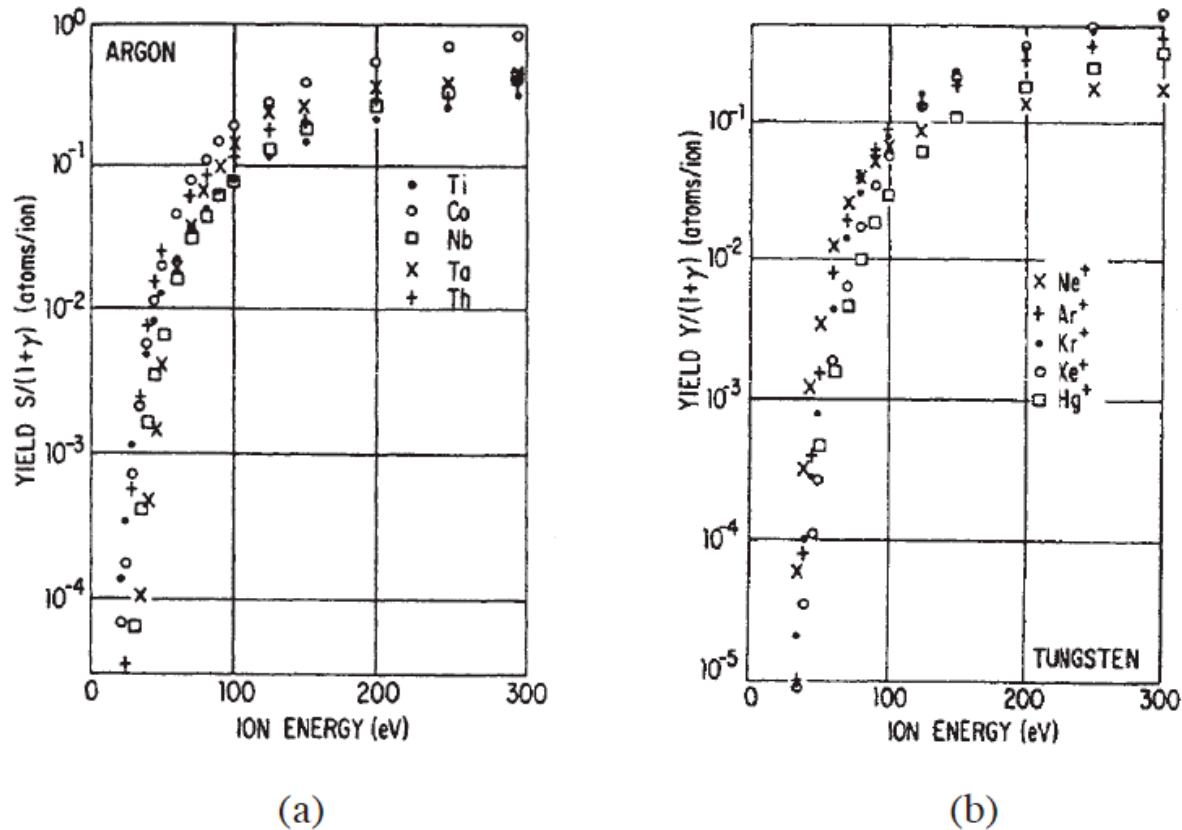


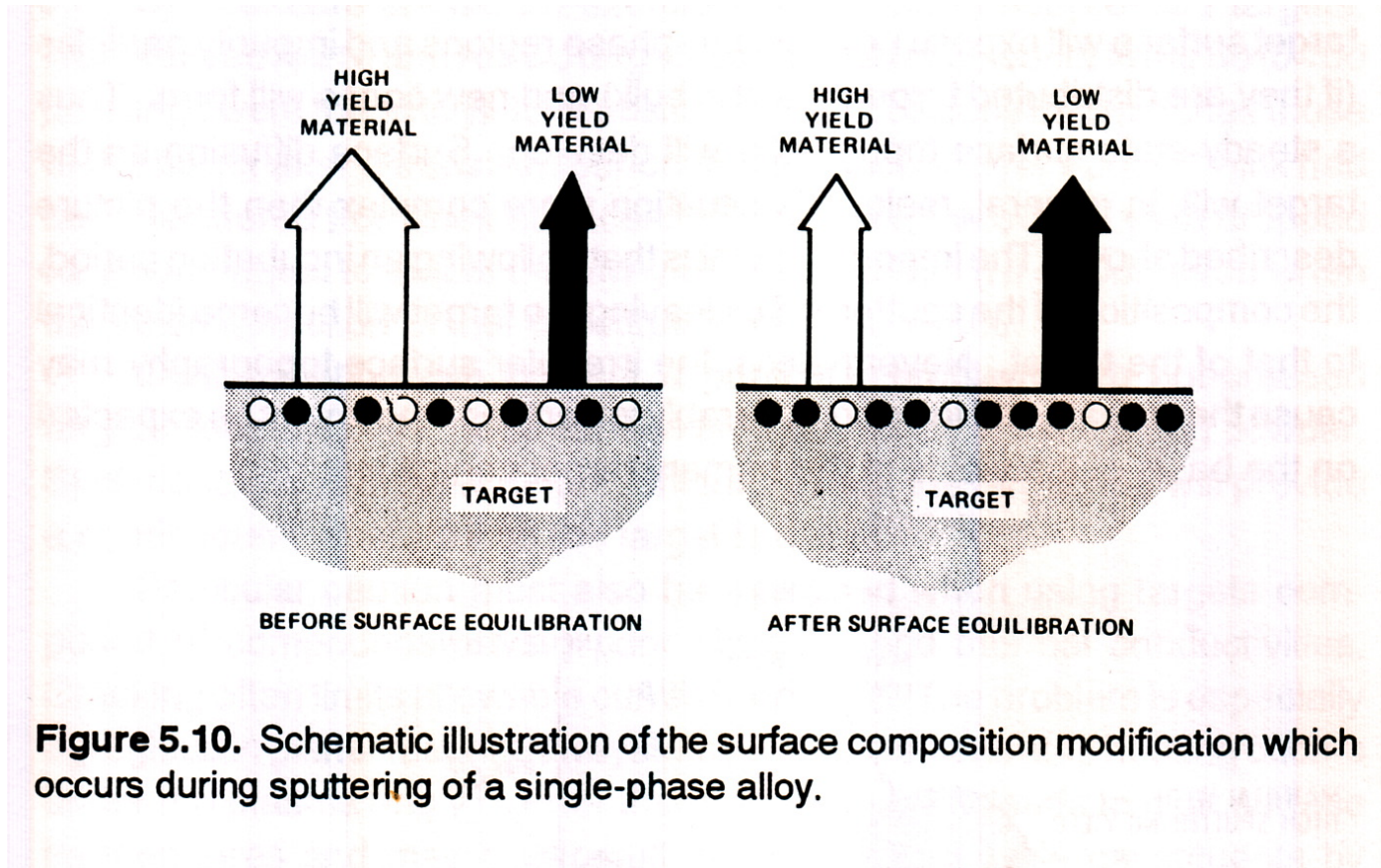
Figure 6-3. Some calculated sputtering yields (adapted from Ref. 20).

# Sputter yield angle dependence and energy distribution



**Figure 3.** Sputter yield,  $S$ , vs ion energy; (a) shown for several materials with Ar<sup>+</sup> bombardment, and (b) for W bombarded by different ion species.<sup>[10]</sup> (Reproduced with permission from Maissel and Glang, Handbook of Thin Film Technology, McGraw-Hill, 1970.)

# Preferential sputtering



**Figure 5.10.** Schematic illustration of the surface composition modification which occurs during sputtering of a single-phase alloy.

# Adatom nucleation and surface diffusion processes

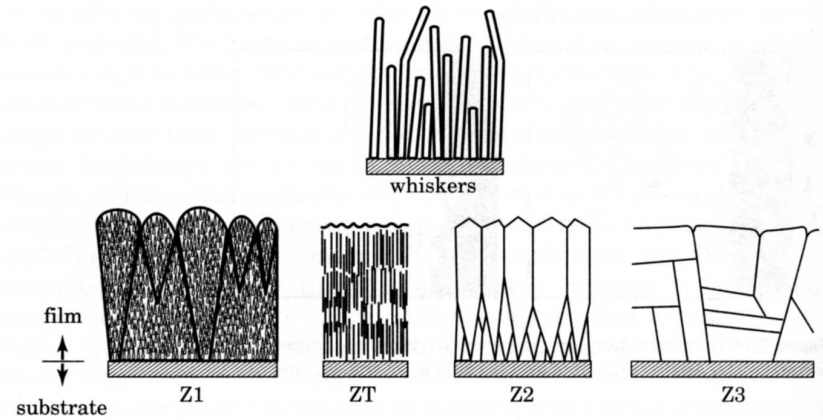
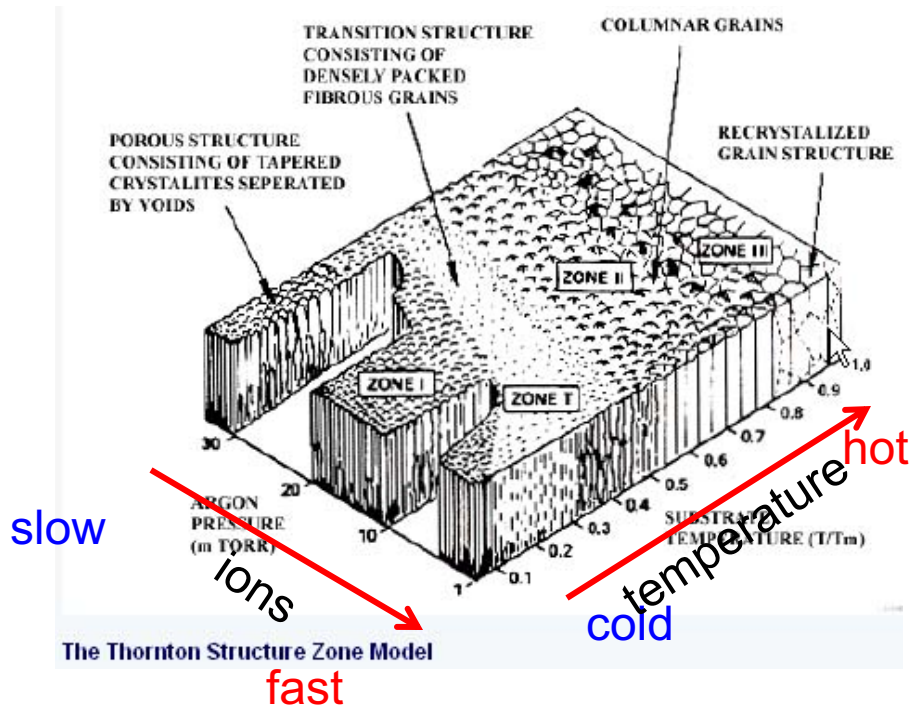
- Shadowing
- Surface diffusion
- Bulk diffusion
- Desorption

## Effecting parameters

- kinetic energy, energy of ions and atoms
- thermal energy
- potential energies
- angle of incidence, topography
- impurities – contamination



# Coating structure and plasma parameters



**Figure 5.15** Characteristics of the four basic structural zones and of whiskers, in cross section. The ratio of substrate T to film melting T ( $T_s/T_m$ ) increases in the direction Z1 → ZT → Z2 → Z3.



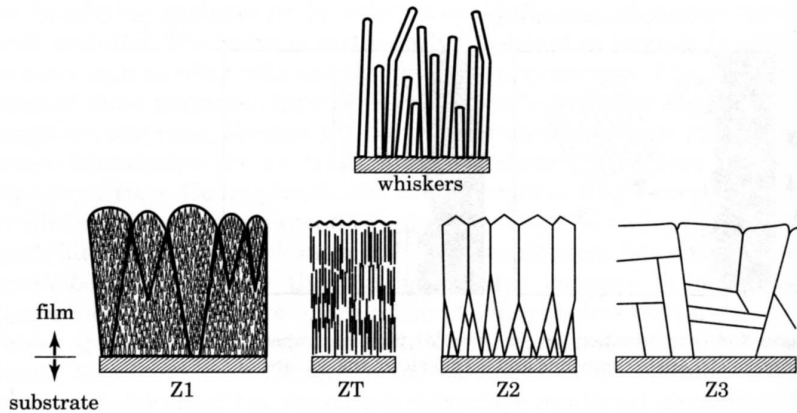


Figure 5.15 Characteristics of the four basic structural zones and of whiskers, in cross section. The ratio of substrate T to film melting T ( $T_s/T_m$ ) increases in the direction  $Z1 \rightarrow ZT \rightarrow Z2 \rightarrow Z3$ .

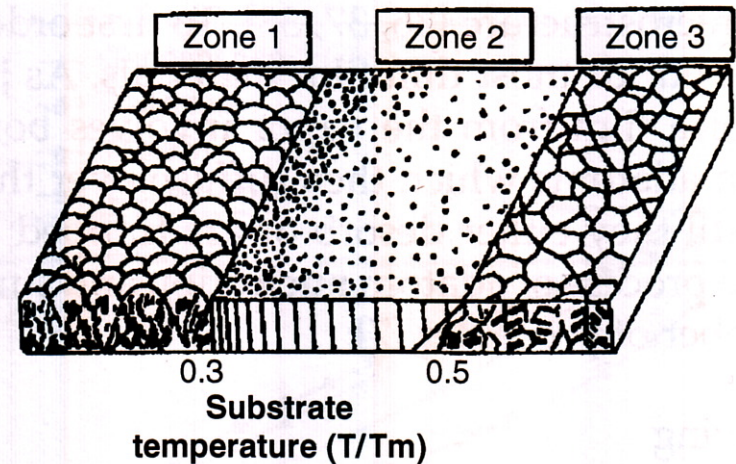


Figure 3.26 Structure zone model of Movechan and Demchishin [39].

## Zone 1

- atomic shadowing, low mobility of atoms, continued nucleation
- fibrous grains, pointing at direction of arriving vapor flux, ending with domes shape
- high density of lattice imperfections and pores at grain boundaries
-

# Shadow effect

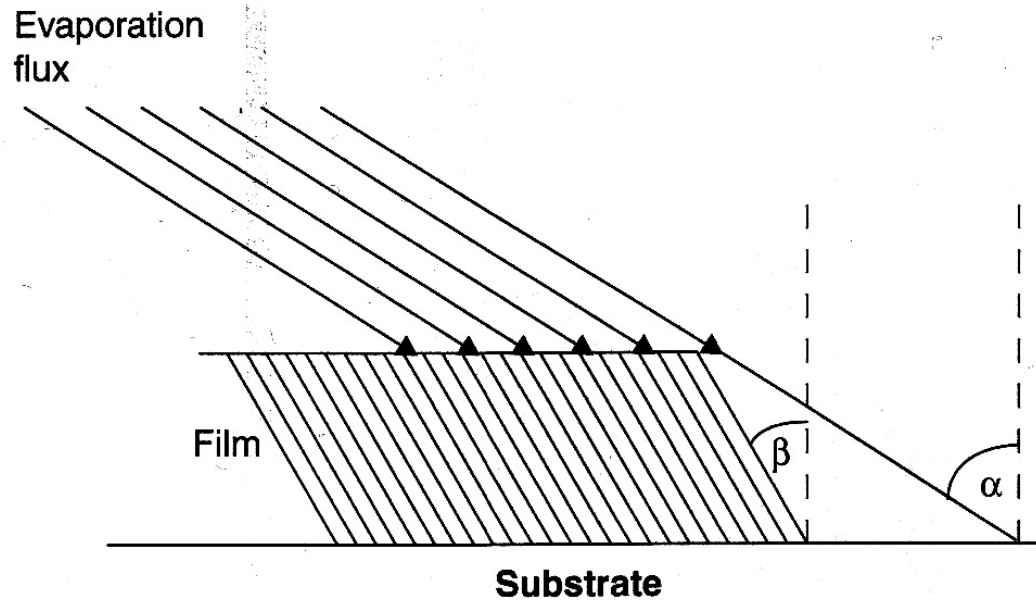
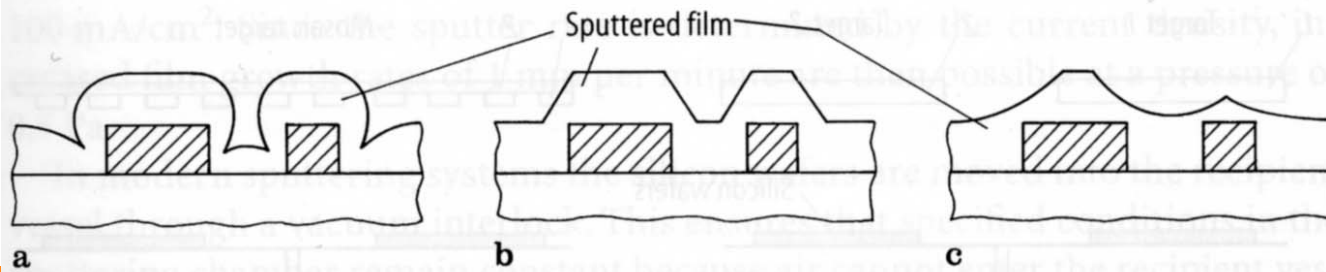


Figure 3.20 Geometry used in the tangent rule [29].



6.2.2012 Koskinen



**Fig. 3.1.19a-c.** Edge coverage of sputtered layers: **a** no bias; **b** moderate bias; **c** heavily biased



# Structural hierarchy

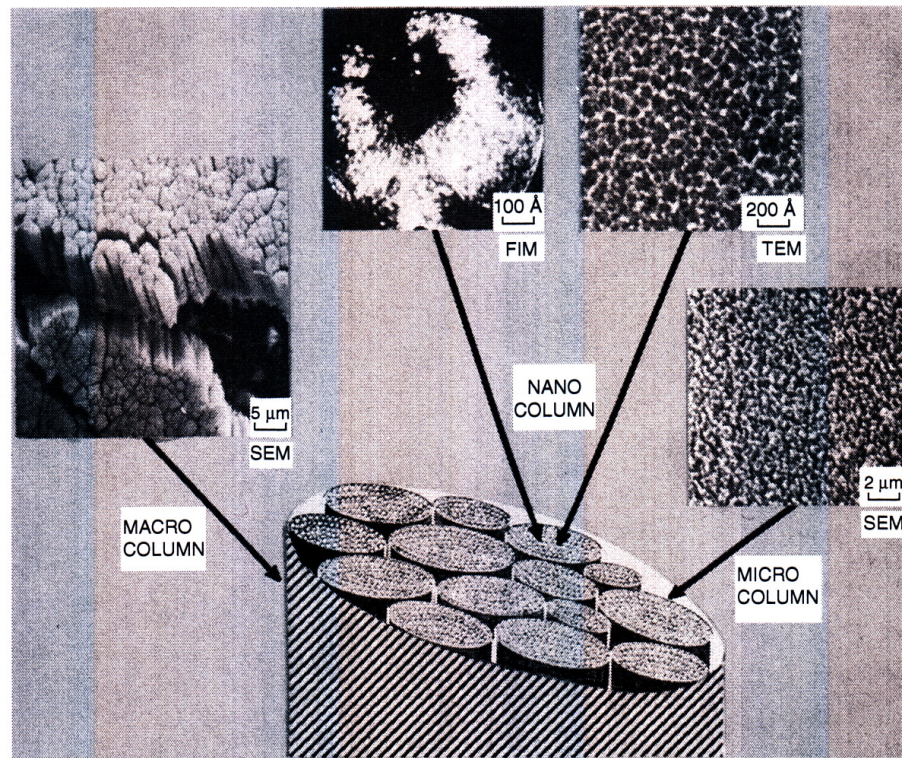


Figure 3.22 Physical structure of nano-, micro and macro columns in a-Ge films [31].

# Nodules

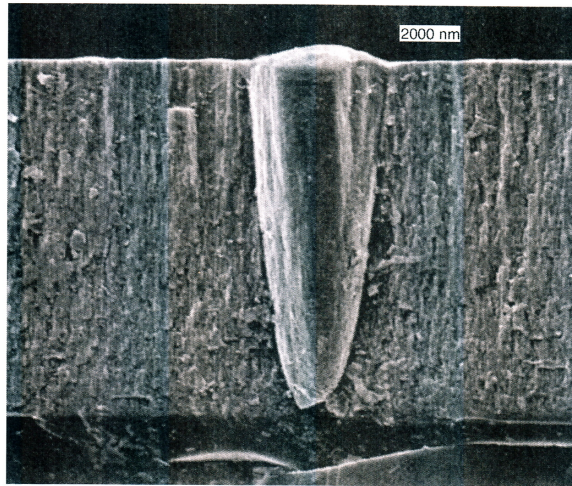


Figure 3.23 Nodule in and AlON rugate filter [28].

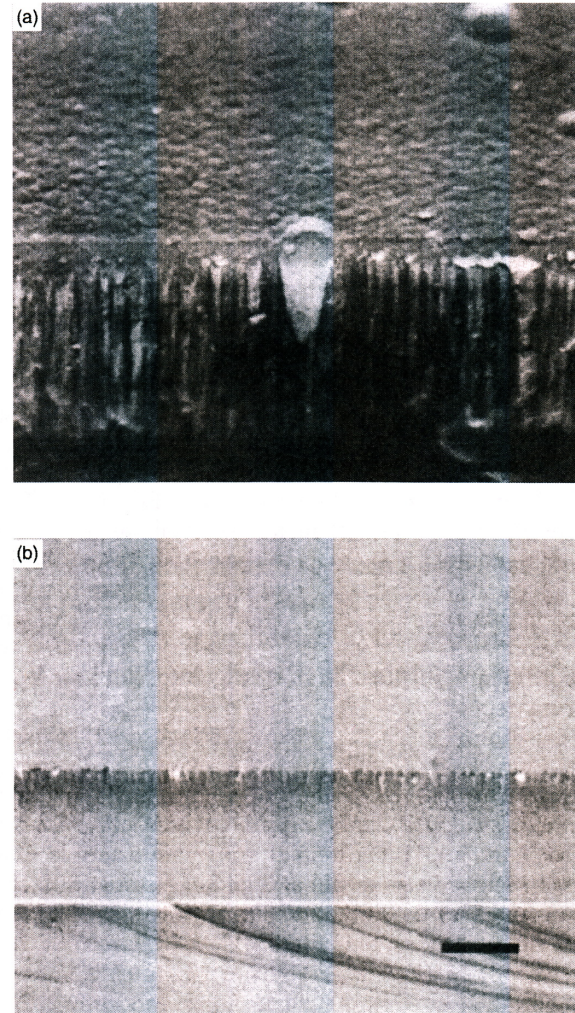


Figure 3.21 SEM micrograph of two SiC films; film (a) had no ion bombardment and film (b) was exposed to ion bombardment [31].



# GLAD

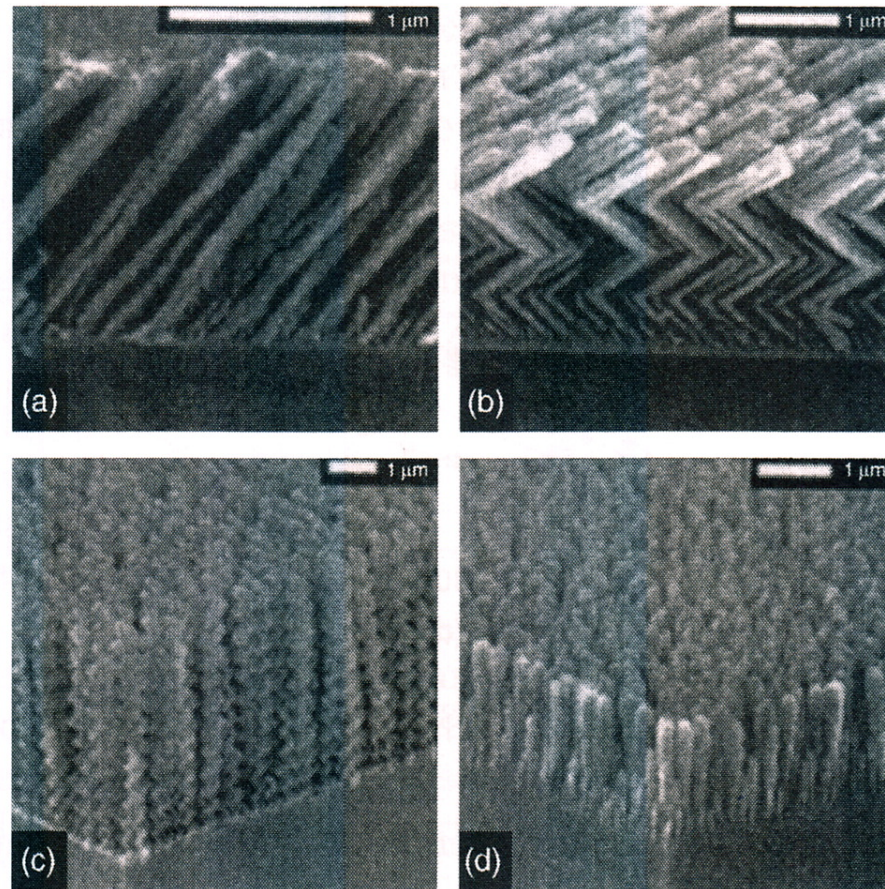
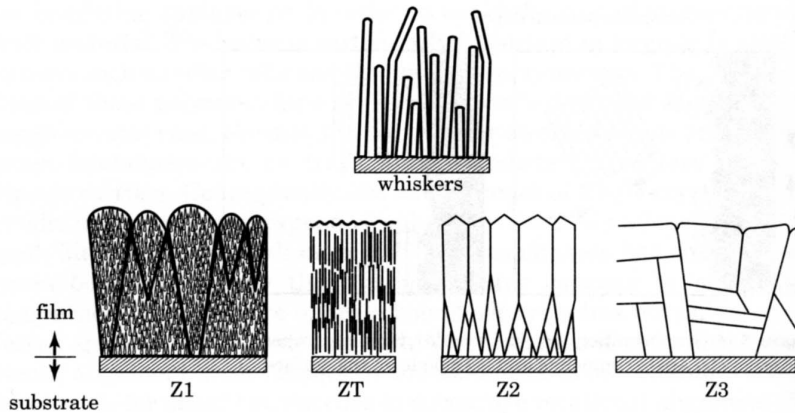
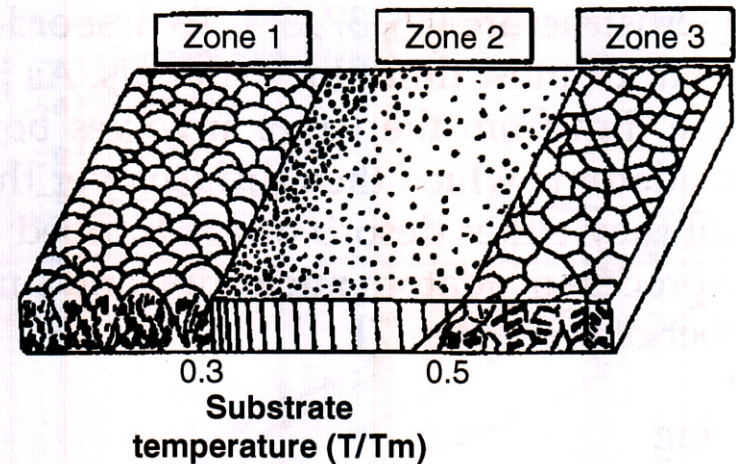


Figure 3.24 Columnar structures fabricated using the GLAD process [32].



**Figure 5.15** Characteristics of the four basic structural zones and of whiskers, in cross section. The ratio of substrate  $T$  to film melting  $T$  ( $T_s/T_m$ ) increases in the direction  $Z1 \rightarrow ZT \rightarrow Z2 \rightarrow Z3$ .



**Figure 3.26** Structure zone model of Movechan and Demchishin [39].

### Zone 2

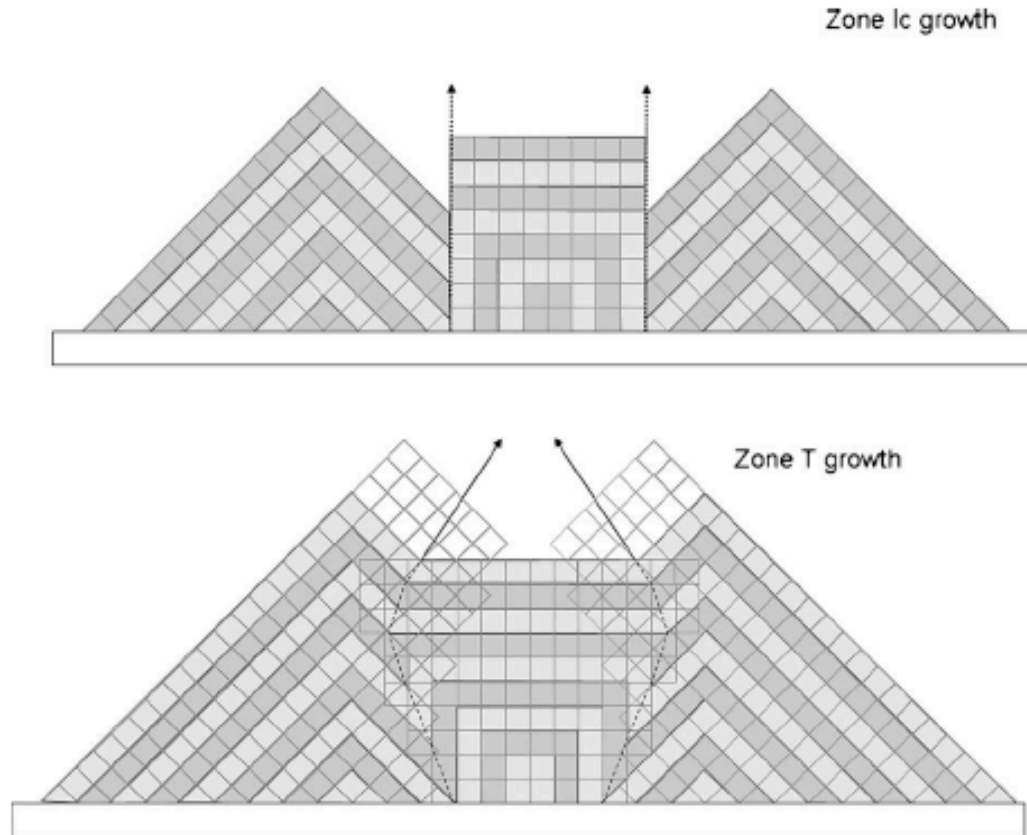
- surface diffusion dominates
- uniform columnar grains, grainsize increases with  $T_h$
- faceted surface
- mechanically weak
- electrically favorable e.g. in piezo electrical thin films

### Zone T

- transition between zone1 and 2 surface diffusion is is “remarkable”
- grain boundary diffusion is limited
- competitive grain growth of V-shaped crystals
- mechanically favorable

# Competition of growing crystals

Handbook of Deposition Technologies for Films and Coatings - Science, Applications and Technology (3rd Edition)  
Edited by: Martin, Peter M. © 2010 William Andrew Publishing



**Figure 5.21: Schematic comparison between zone Ic and zone T growth. To indicate the identical normal growth rate of the planes of both grains, alternating coloring is used. In zone T, an overgrowth of one grain by an adjacent grain is observed.**



# Columnar growth

AlN piezoelectric film

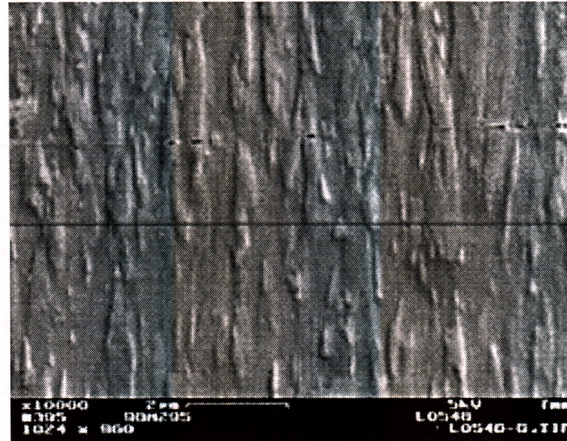


Figure 3.18 SEM picture of well-behaved columnar thin film microstructure.

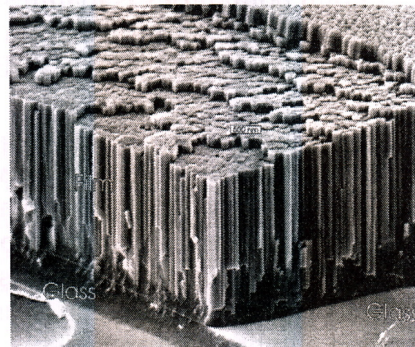


Figure 3.19 Columnar structure in an RF sputtered ALON film [28].

# Columnar crystals





# Columnar crystals



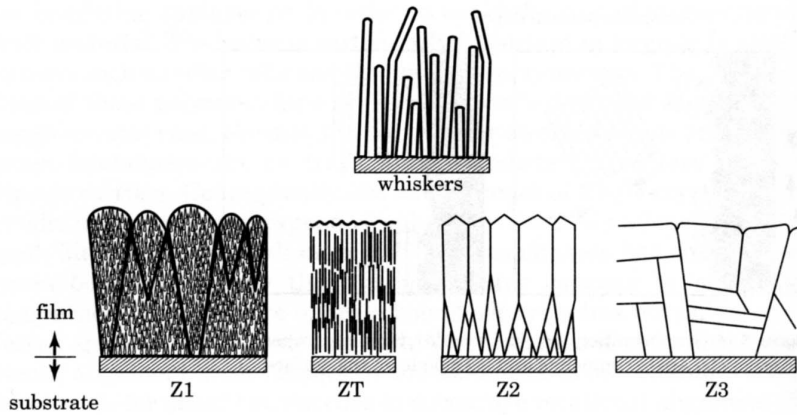


Figure 5.15 Characteristics of the four basic structural zones and of whiskers, in cross section. The ratio of substrate  $T$  to film melting  $T$  ( $T_s/T_m$ ) increases in the direction  $Z1 \rightarrow ZT \rightarrow Z2 \rightarrow Z3$ .

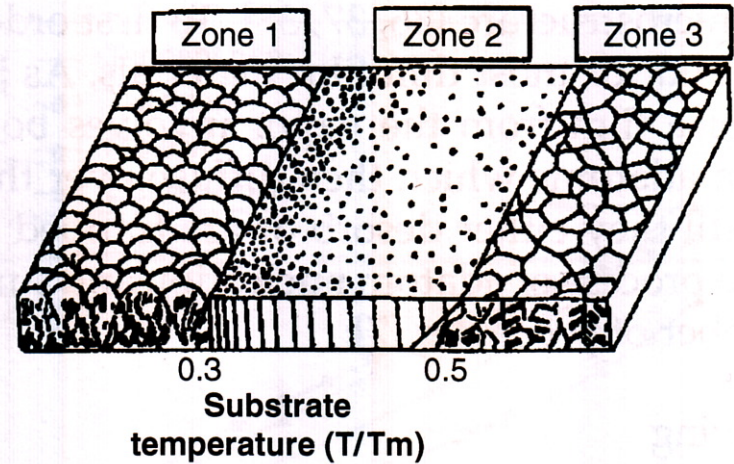


Figure 3.26 Structure zone model of Movechan and Demchishin [39].

### Zone 3

- bulk diffusion dominates
- recrystallization of large crystals



# Effect of ion energy

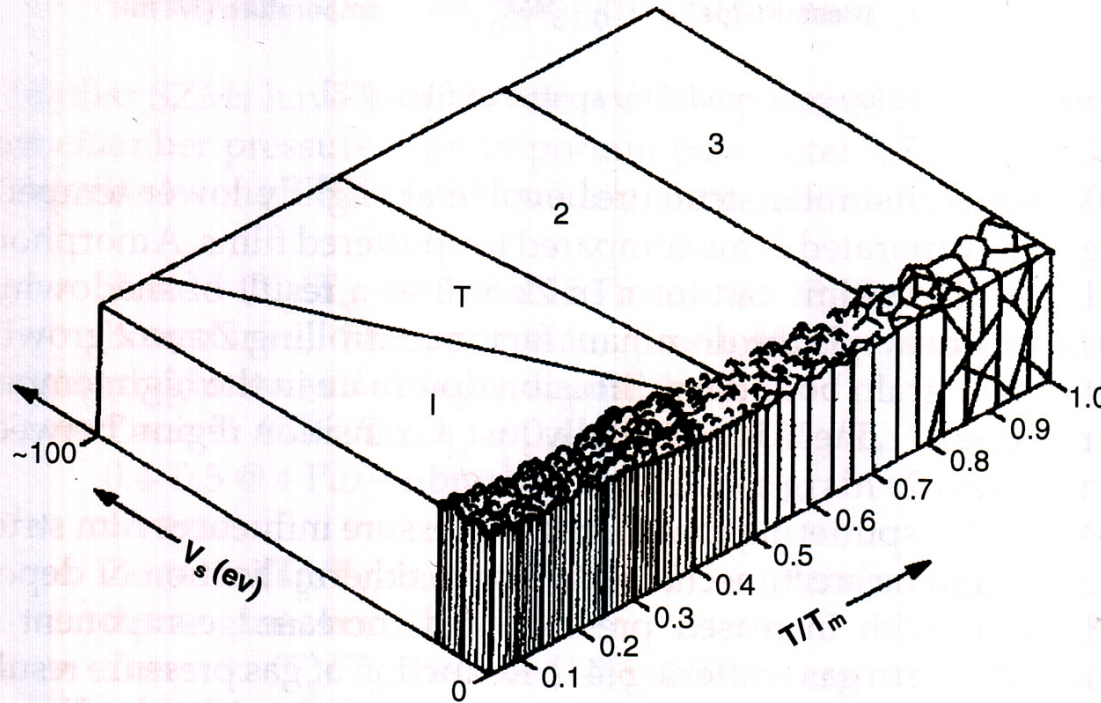


Figure 3.28 Revised SZD for RF sputtering, including ion bombardment.

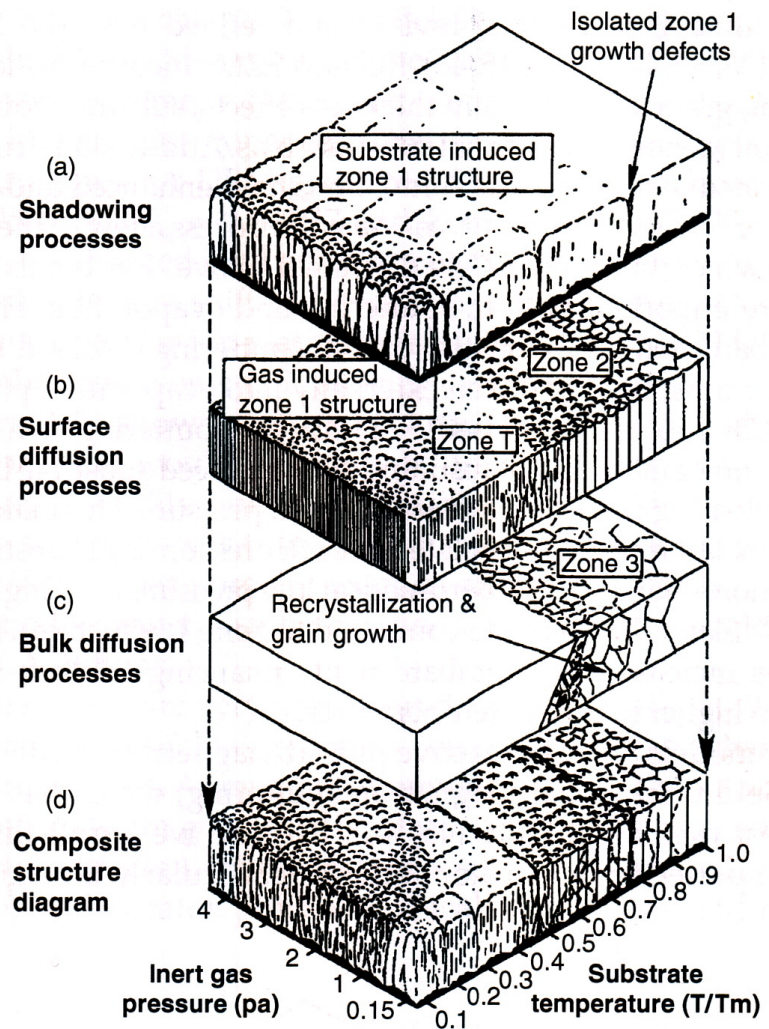


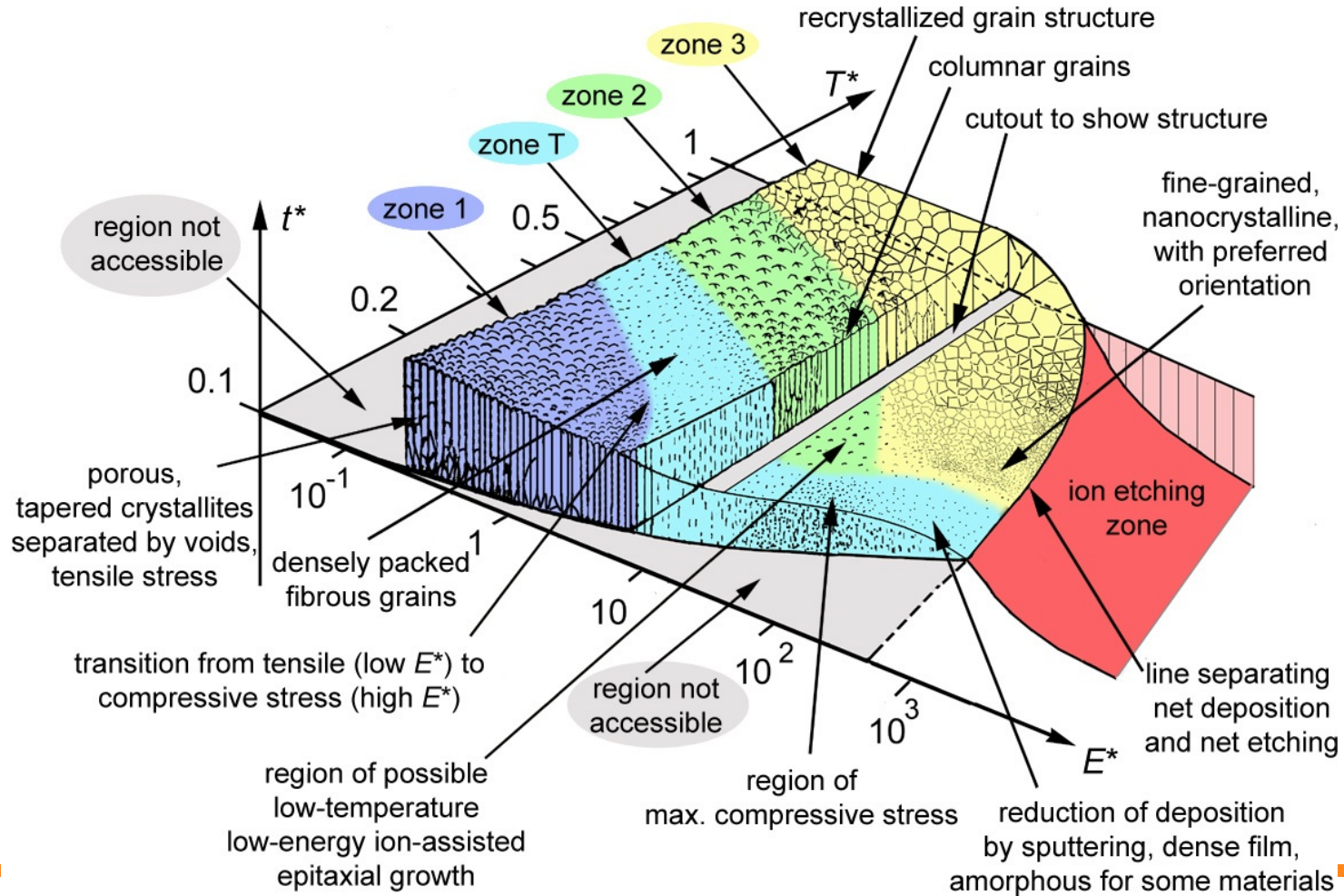
Figure 3.27 Structure zone model for sputtered films [37].

# Generalize parameters to all PVD processes

- Replace the linear  $T_h$  axis with a generalized temperature  $T^*$ , which includes the homologous temperature + the temperature shift caused by the potential energy of particles arriving on the surface (i.e., energetic particle and ion bombardment).
- Replace the linear pressure axis with a logarithmic axis for a normalized energy  $E^*$ , which encompasses displacement and heating effects caused by the kinetic energy of bombarding particles.
- Label the z-axis with a net film thickness  $t^*$  which will allow maintenance of film structure while including the effects of thickness reduction by densification and sputtering. Ion etching is included in this quantity.



# Modified Thornton diagram





# Reduced parameters SZD

- $T^* = T_h + T_{\text{pot}}$
- $T_h = T_s/T_m$
- $E_{\text{pot}} = E_c + (E_i - \phi)$
- $E_{\text{kin}} = E_o + QeV_{\text{sheath}}$
- $T_{\text{pot}} = E_{\text{pot}}/kN_{\text{moved}}$
- $t^* = \text{thickness}$

$$E^* = \sum_{\alpha} \frac{E_{\text{kin},\alpha} m_{\alpha}}{E_c m_s} J_{\alpha} / \sum_{\alpha} J_{\alpha}$$

- $T_s$ , substrate temperature
- $T_m$ , melting temperature
- $E_c$  heat of sublimation or cohesive energy (1 – 9 eV/atom)
- $E_i$  ionization energy (4 – 10 eV/atom)
- $E_{\text{kin}}$  ion kinetic energy
- $E_o$  plasma potential
- $V_{\text{sheath}}$  sheath potential
- $\phi$  electron work function (c. 4 eV)
- $J_a$ , flux of species a
- $m_a$ , mass of incoming atom
- $m_s$ , mass of substrate
- $k$ , Boltzmann constant
- $N_{\text{moved}}$ , number of rearranged atoms

# TRIM and SRIM simulations

<http://www.srim.org/SRIM/SRIM%2008.pdf>

The screenshot shows the TRIM Setup Window interface. At the top, it says "TRIM (Setup Window)" and "Type of TRIM Calculation" is set to "Ion Distribution and Quick Calculation of Damage". Below this, there are buttons for "TRIM Demo" and "Restore Last TRIM Data".

The "ION DATA" section shows the ion is Hydrogen (H) with an atomic number of 1, mass of 1.008 amu, and an energy of 10 keV. The angle of incidence is 0 degrees.

The "TARGET DATA" section is titled "Input Elements to Layer 1". It contains a table with columns for Layer Name, Width, Density, Compound, Gas, Symbol, Name, Atomic Number, Weight, Atom Stoich or %, Damage (eV) Disp, and Latt Surf. The table has one row for "Layer 1" with a width of 10000 Angstroms, density of 0, compound of 1, and symbol of H. The damage parameters are 20, 3, and 2.

The "Special Parameters" section includes fields for "Name of Calculation" (H (10) into Layer 1), "Stopping Power Version" (SRIM-2003), "AutoSave at Ion #" (10000), "Total Number of Ions" (99999), and "Random Number Seed".

The "Output Disk Files" section has checkboxes for "Ion Ranges", "Backscattered Ions", "Transmitted Ions/Recoils", "Sputtered Atoms", and "Collision Details". There are also options to "Resume saved TRIM calc." and "Use TRIM-96 (DOS)".

At the bottom, there are buttons for "Save Input & Run TRIM", "Clear All", "Calculate Quick Range Table", "Main Menu", "Problem Solving", and "Quit".