Aalto University
School of Chemical
Technology

CHEM E5125 Thin Film Technology

Lecture 3 PVD 1

Plasma and ion bombardment

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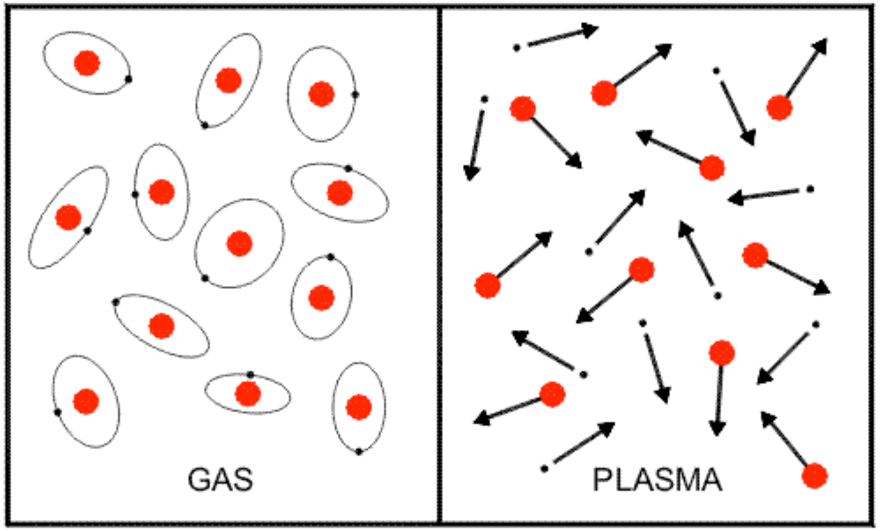
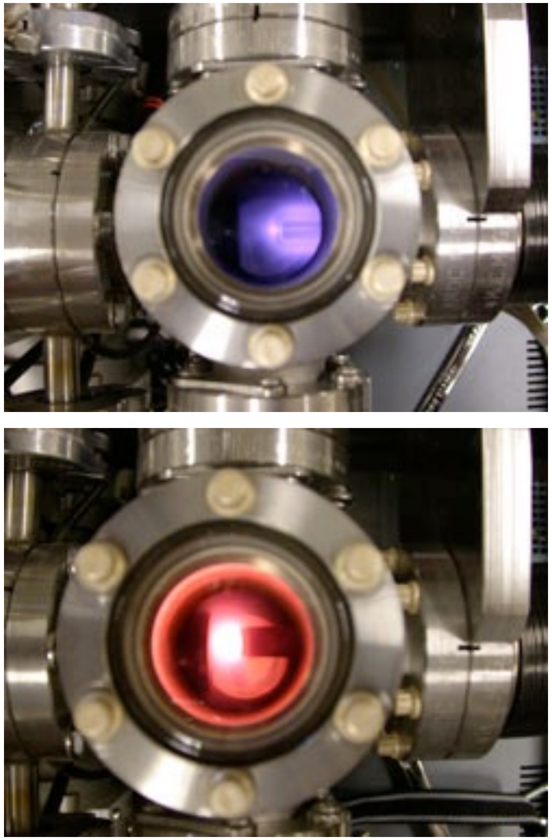
Contents

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

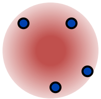
Plasma

- 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
  -

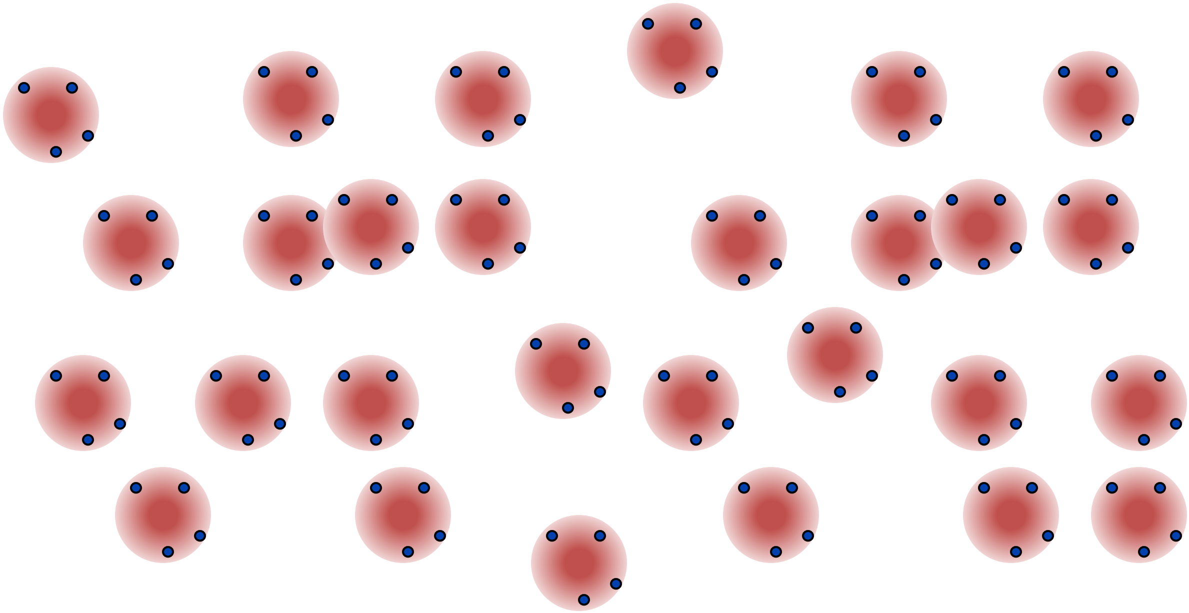




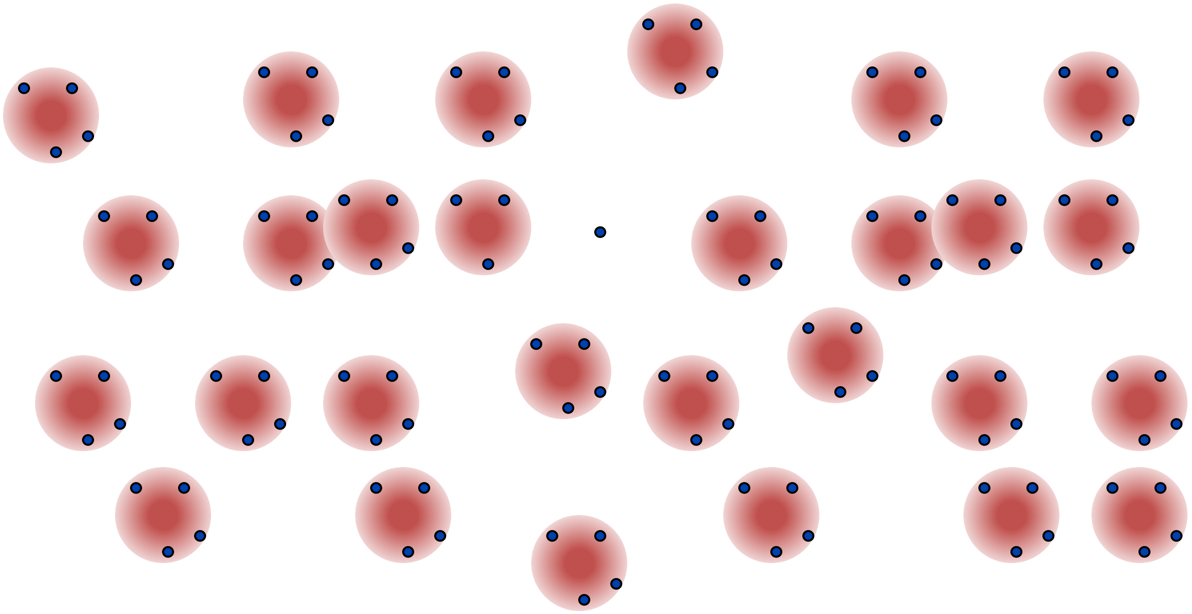
Glow discharge



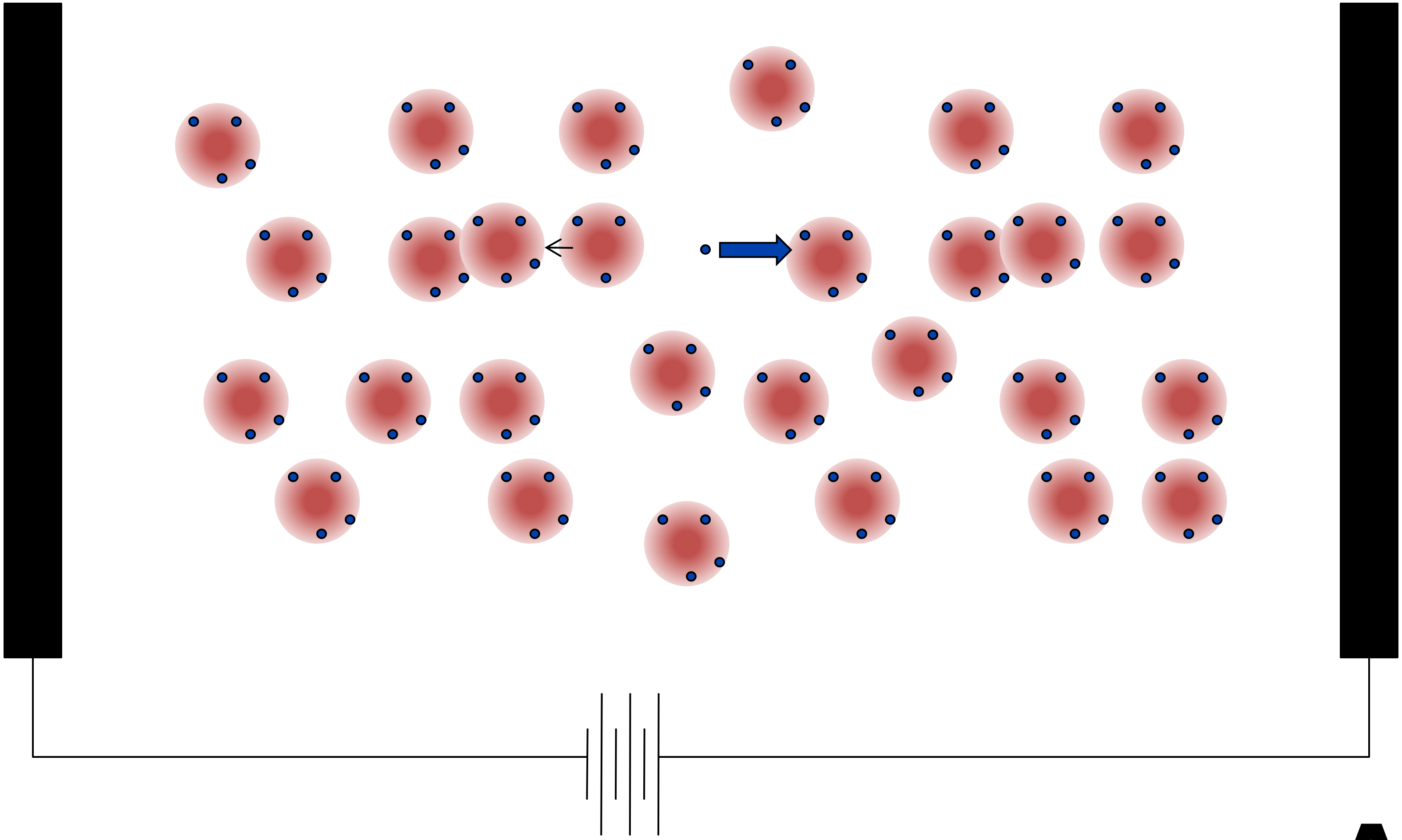
Glow discharge



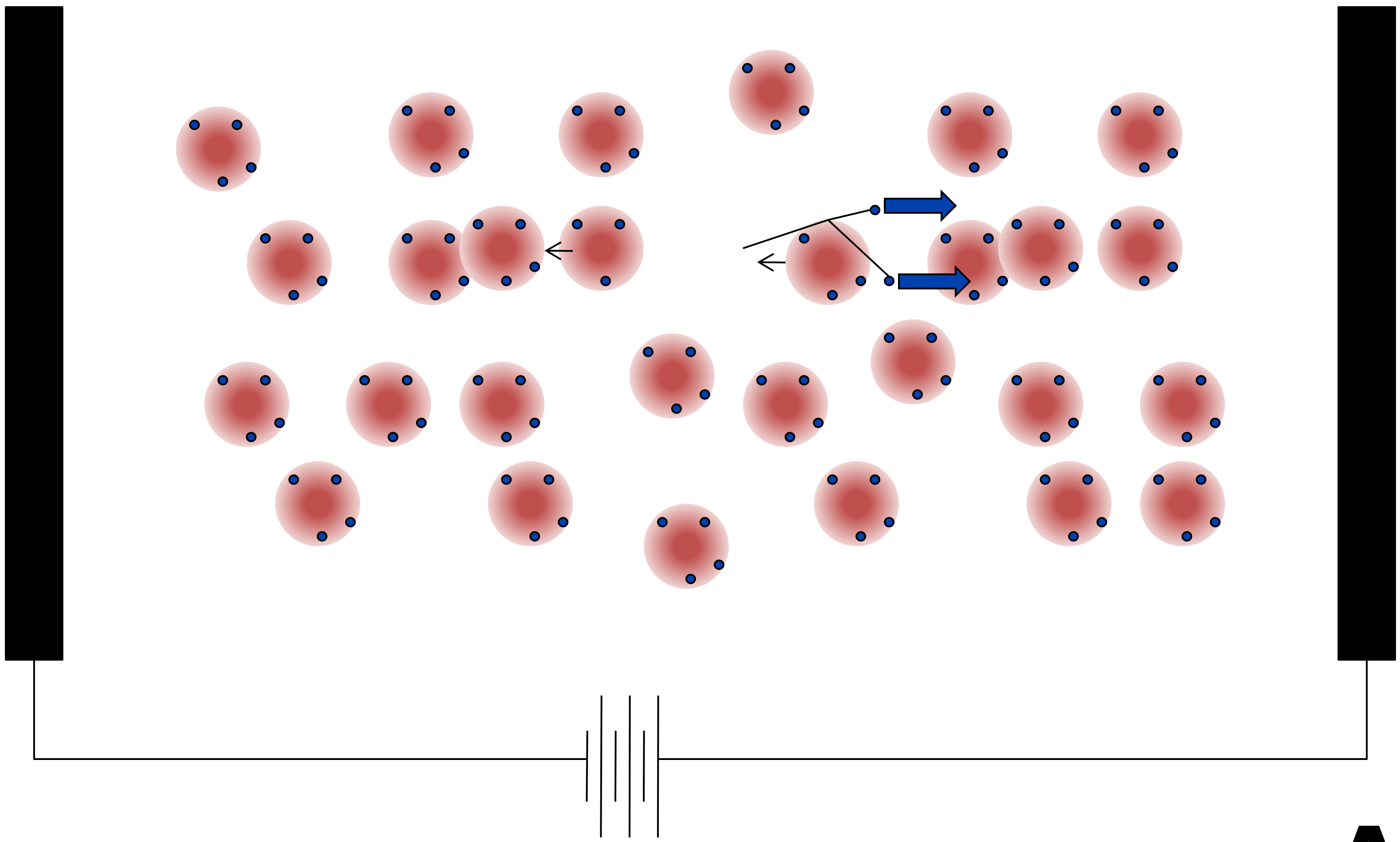
Glow discharge



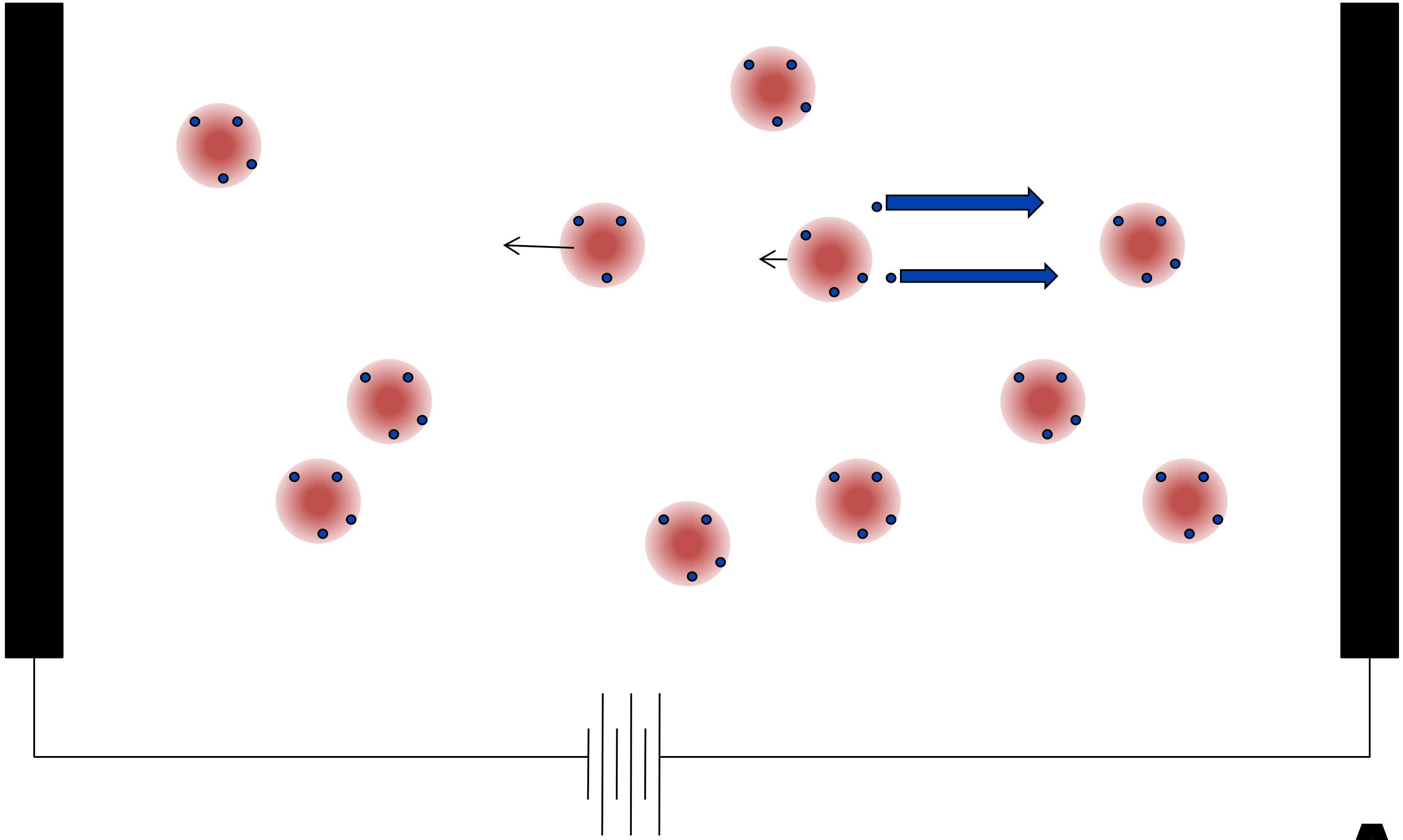
Glow discharge



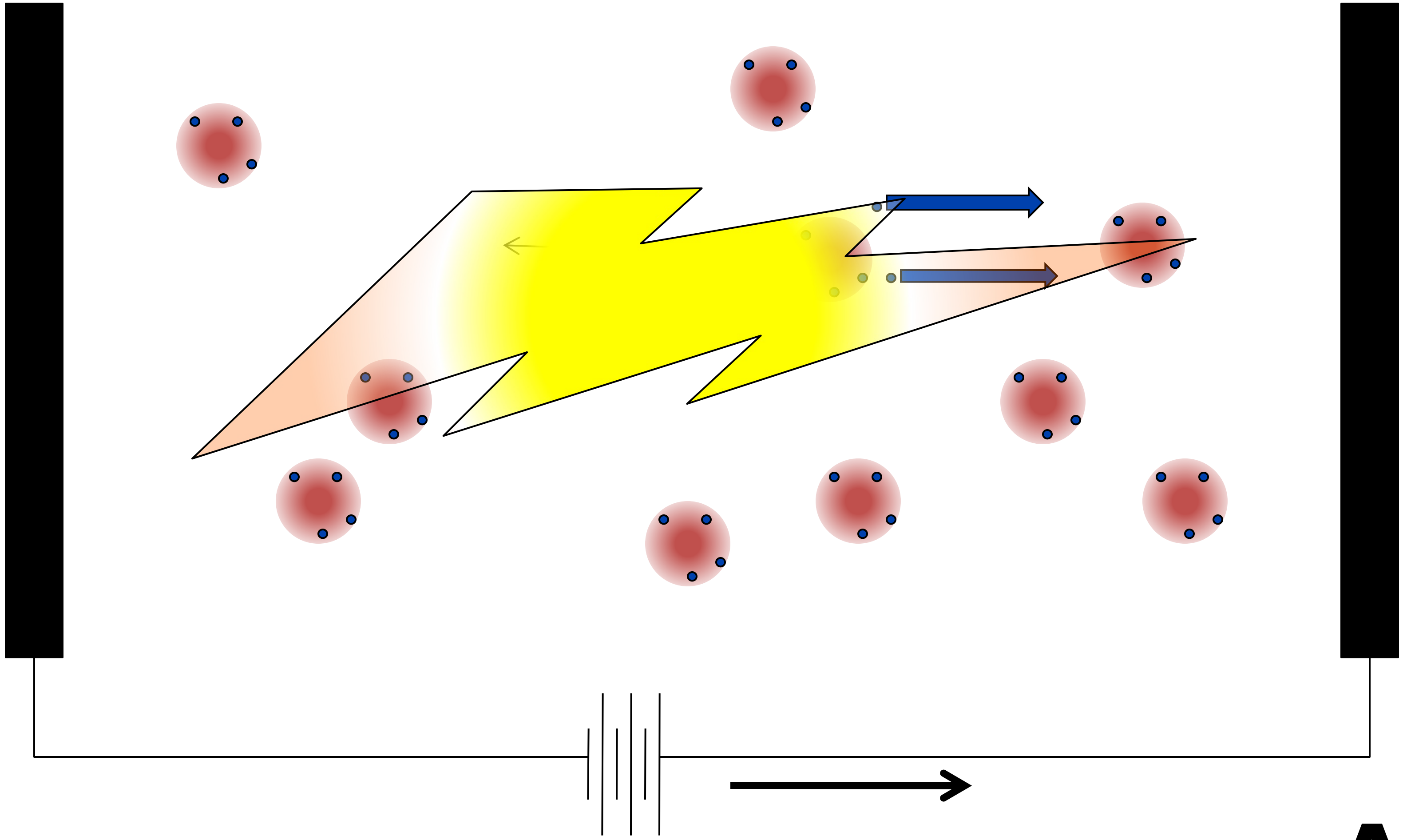
Glow discharge



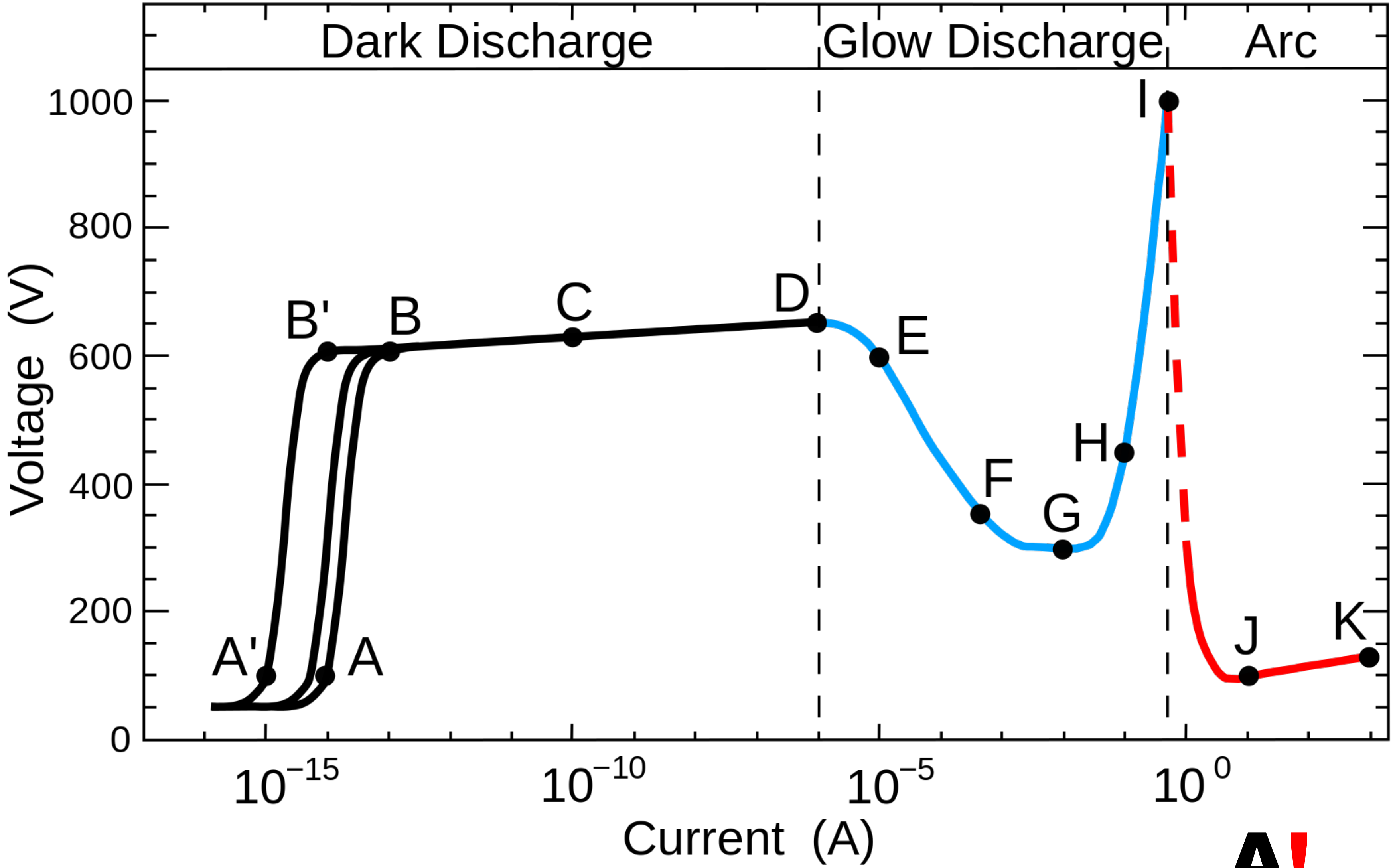
Glow discharge



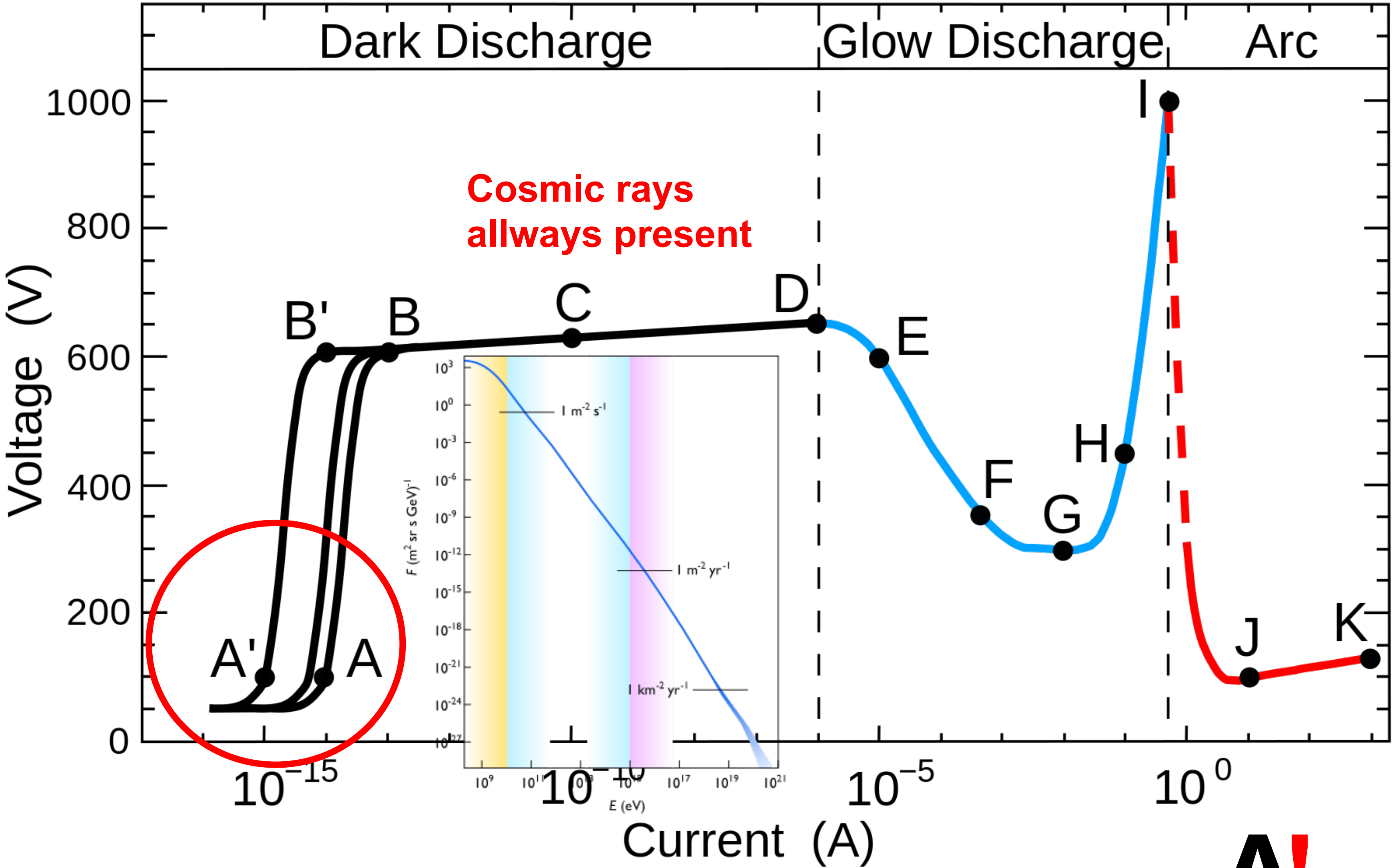
Glow discharge



DC Plasma glow discharge and arc

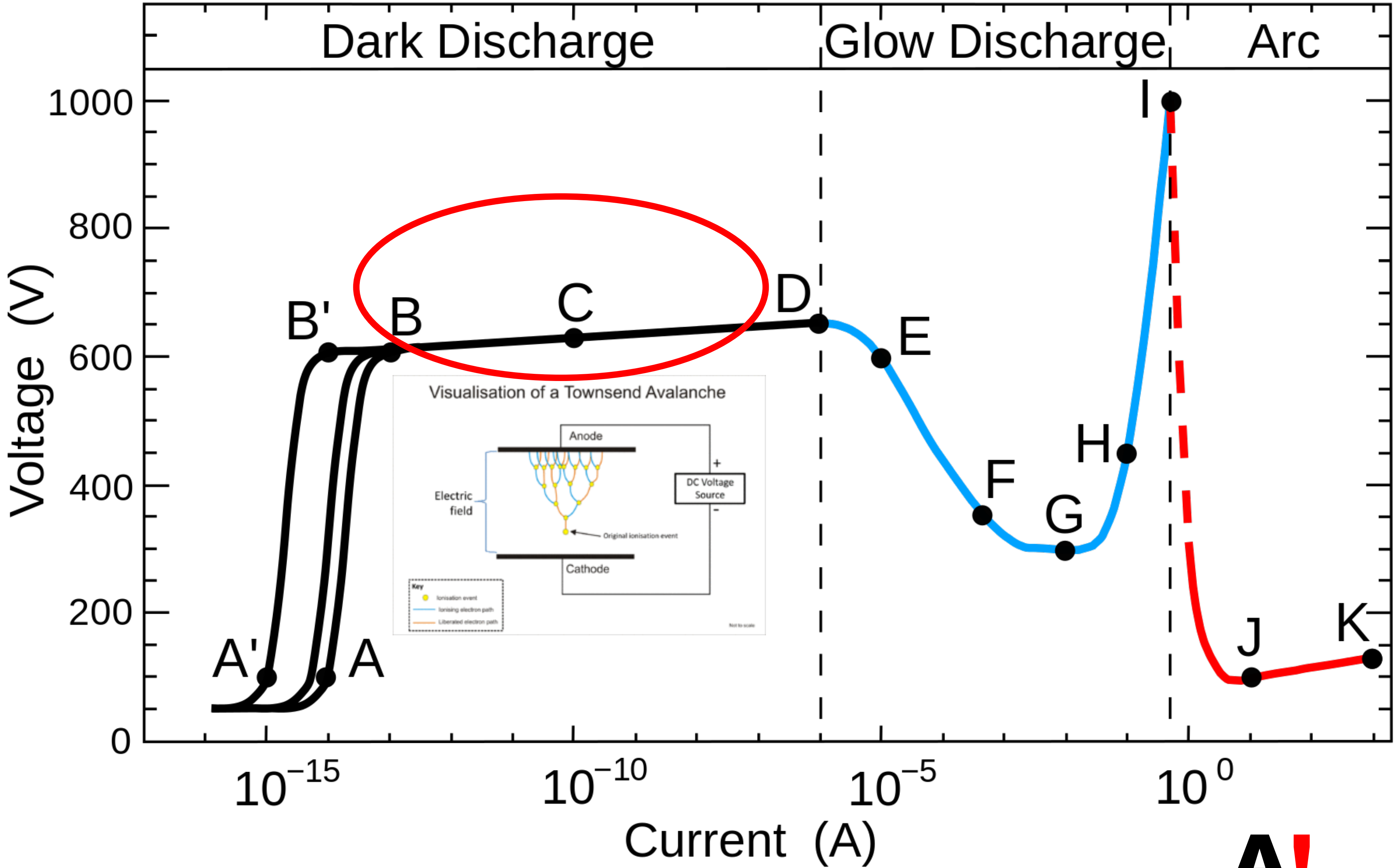


DC Plasma glow discharge and arc

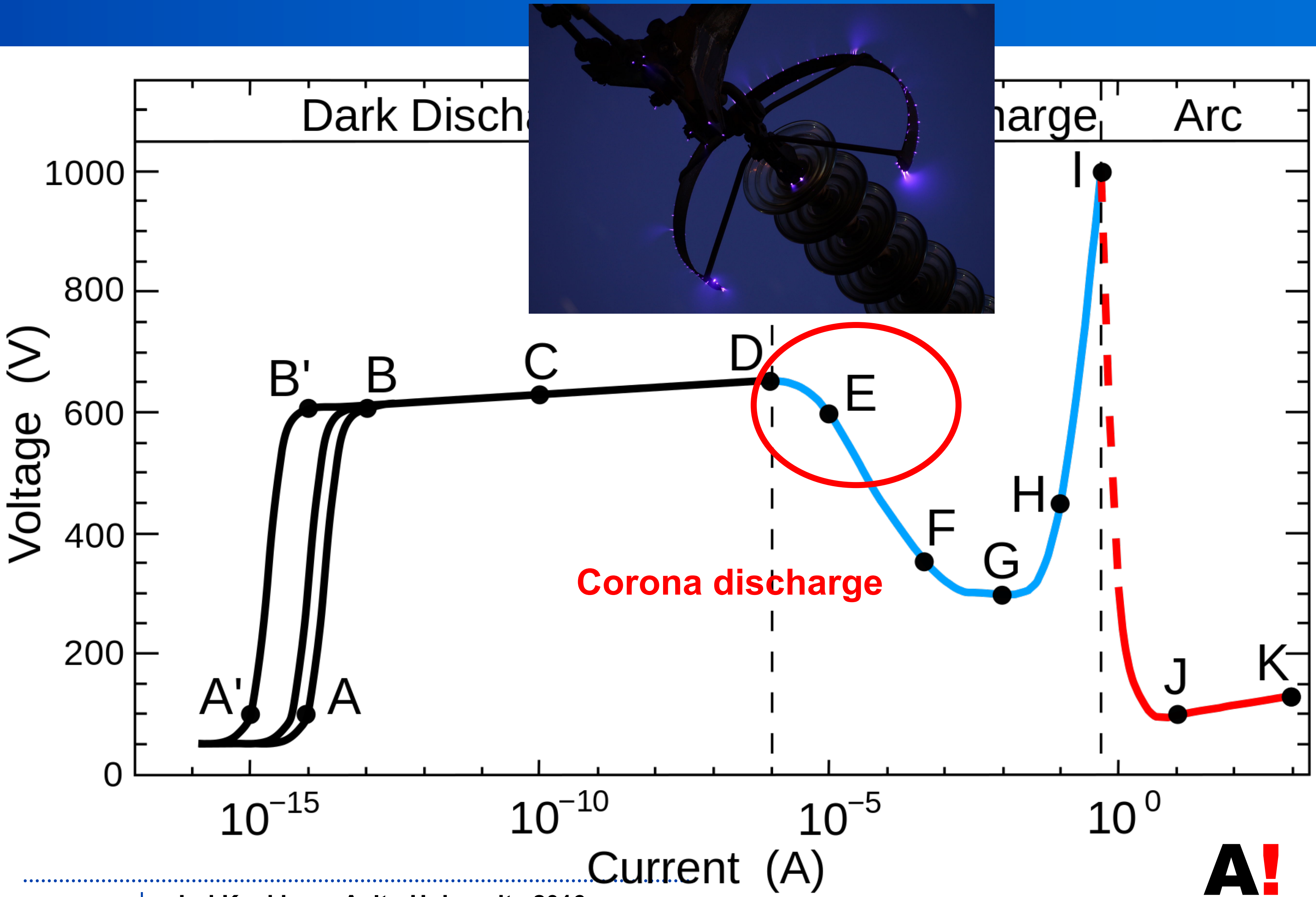


Cosmic rays allways present

DC Plasma glow discharge and arc

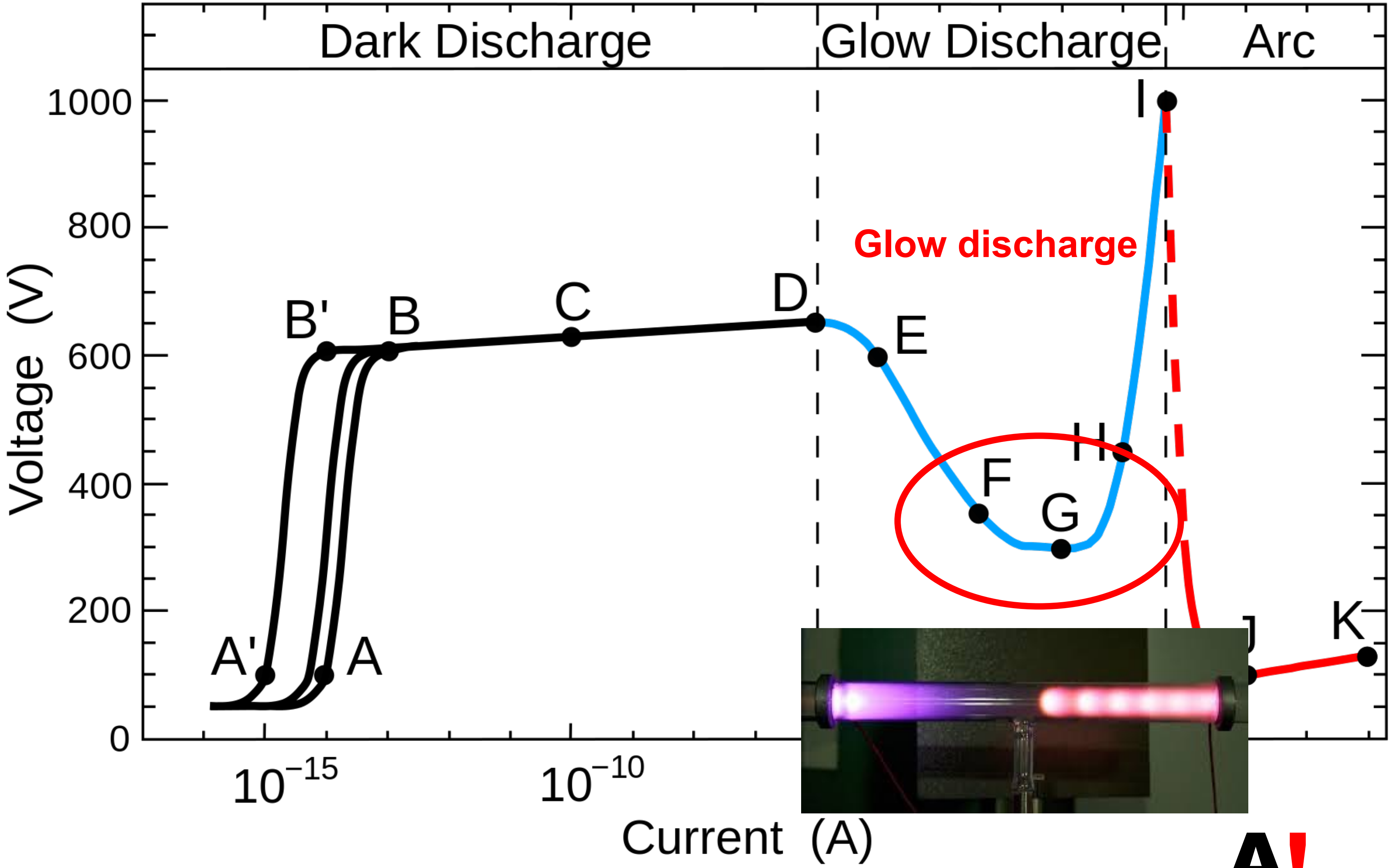


DC Plasma glow discharge and arc

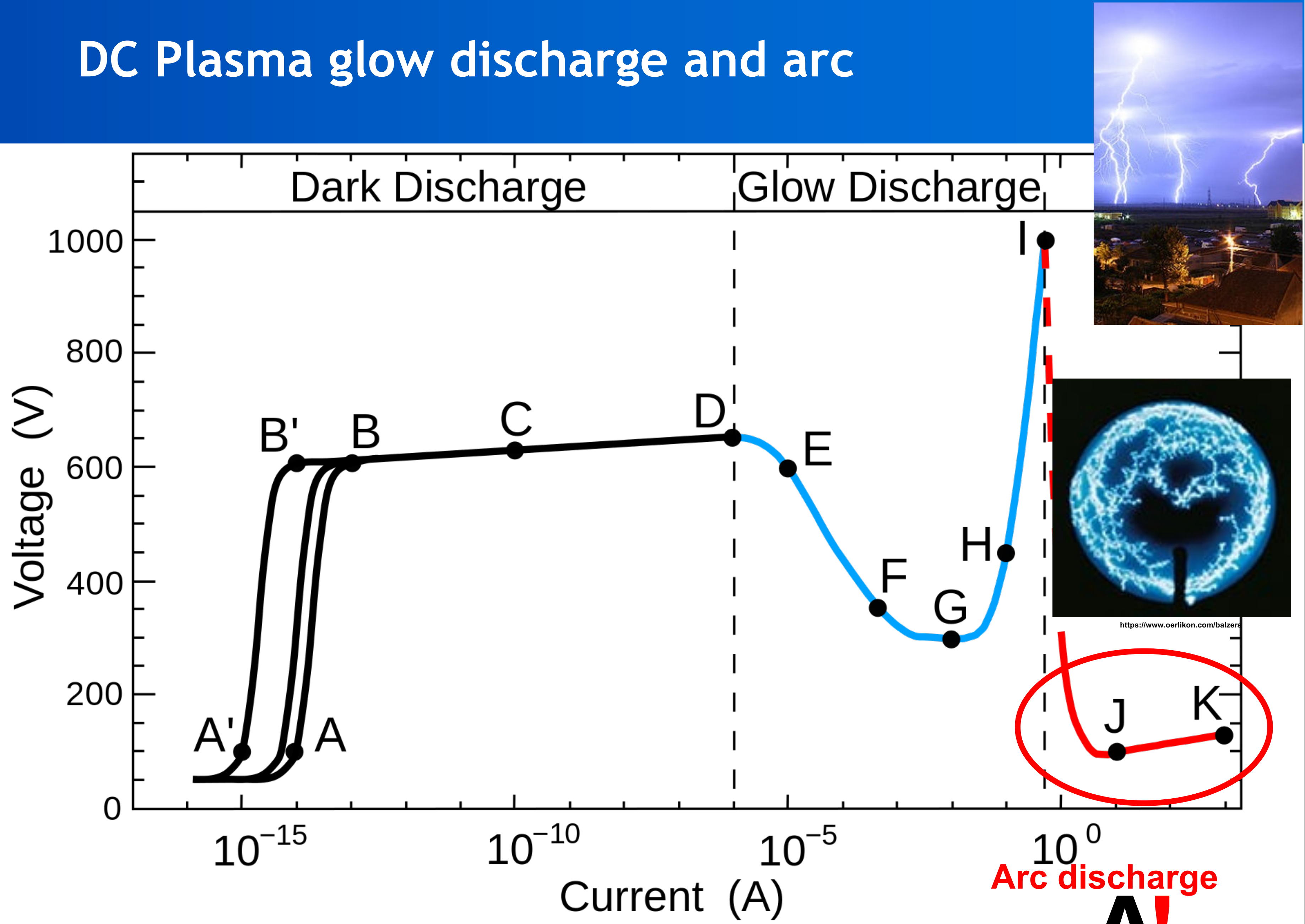


Corona discharge

DC Plasma glow discharge and arc

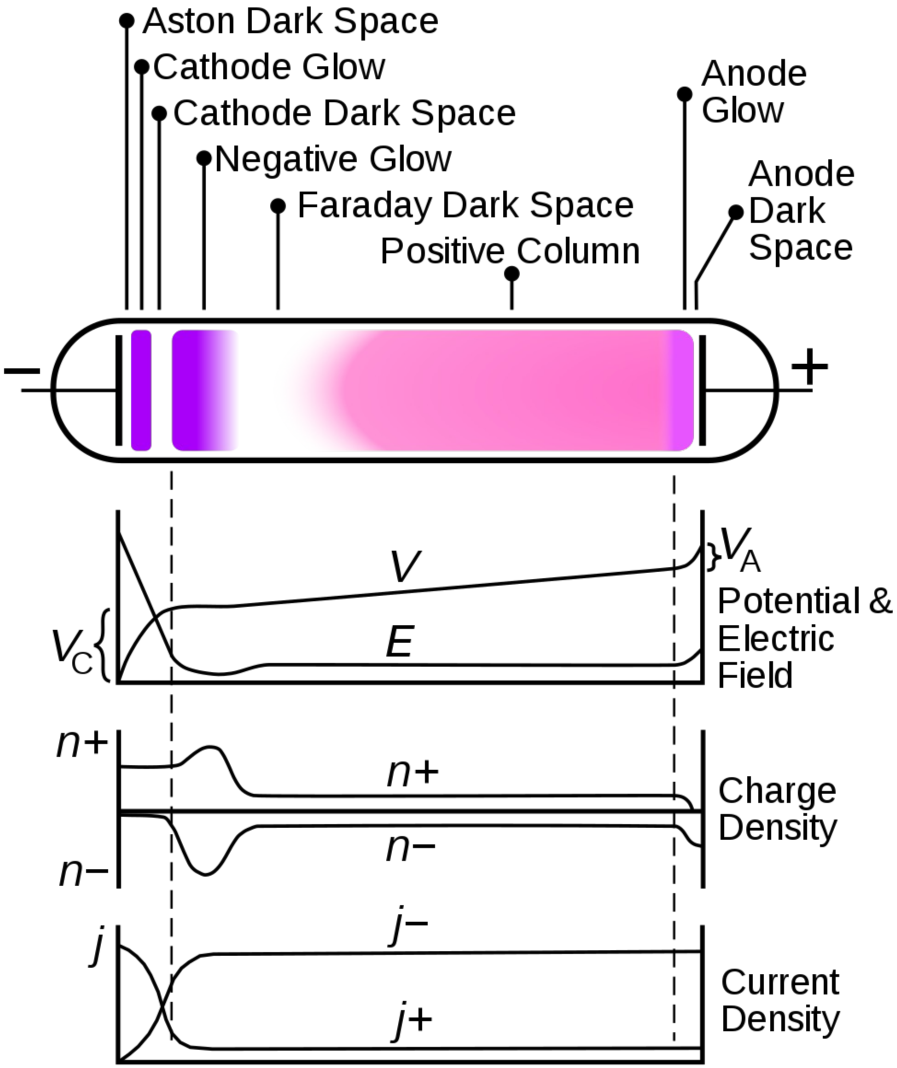


DC Plasma glow discharge and arc



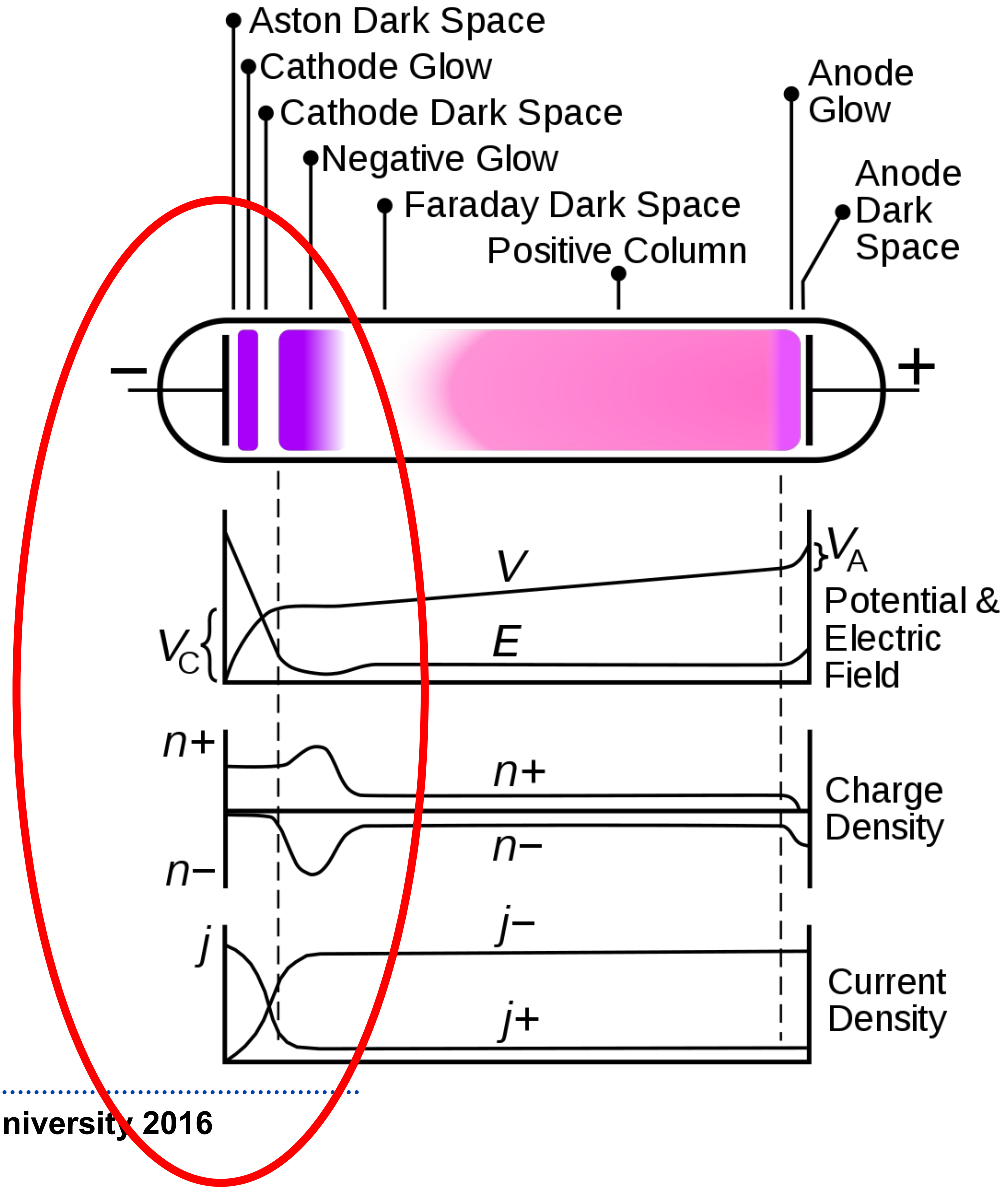
https://www.oerlikon.com/balzers

Glow discharge plasma

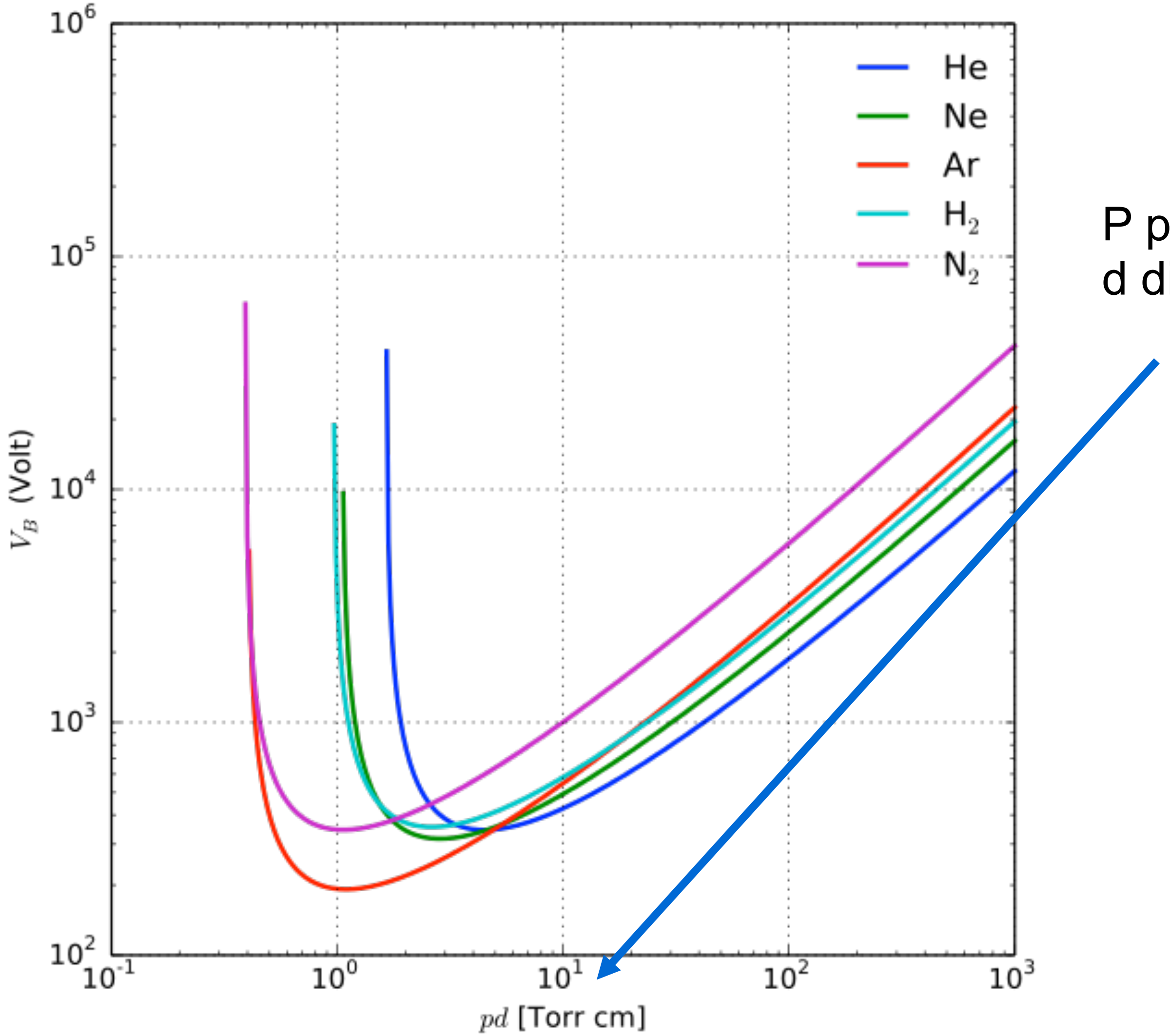


Glow discharge plasma

For PVD
Interesting things
happen
here

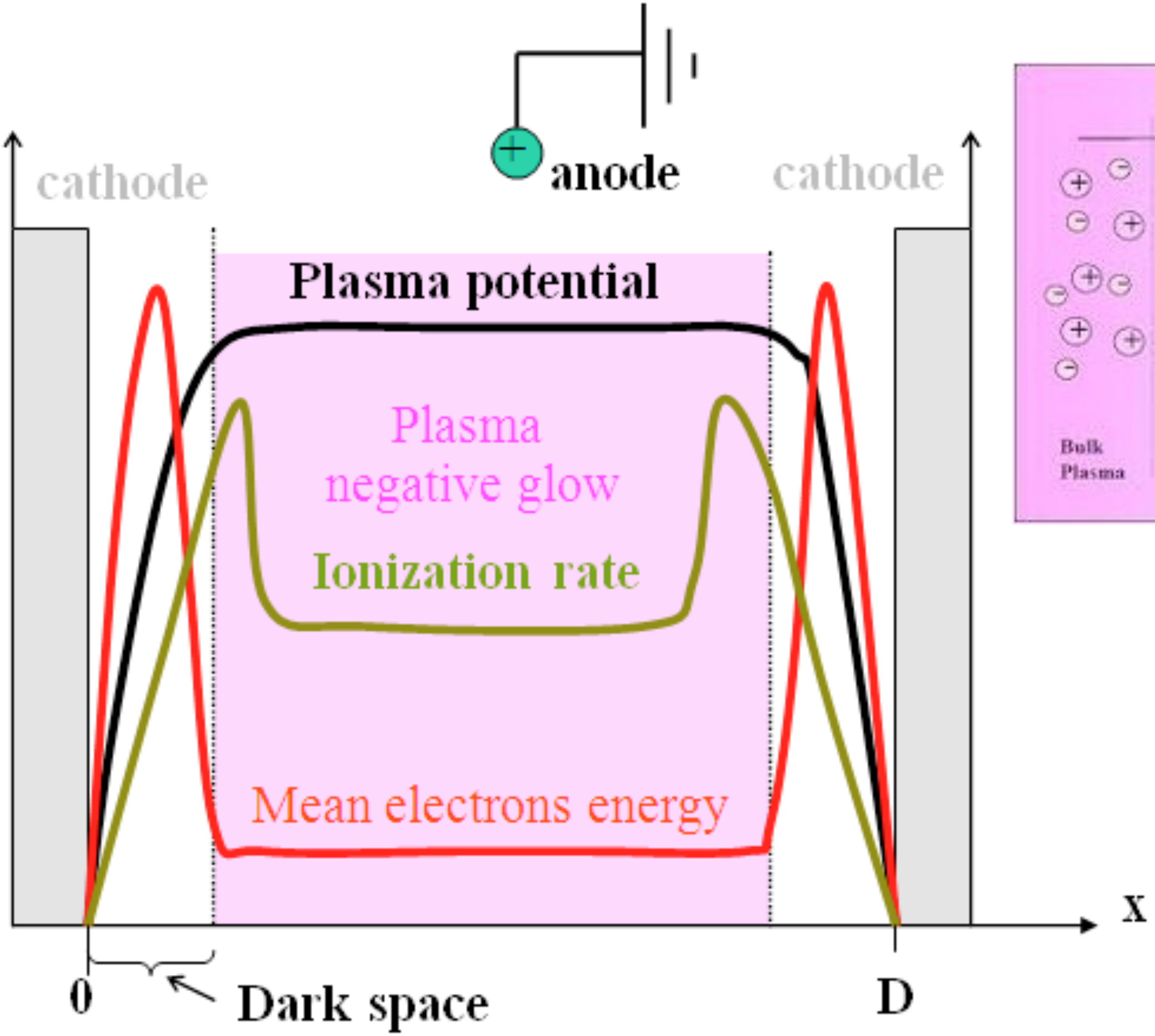


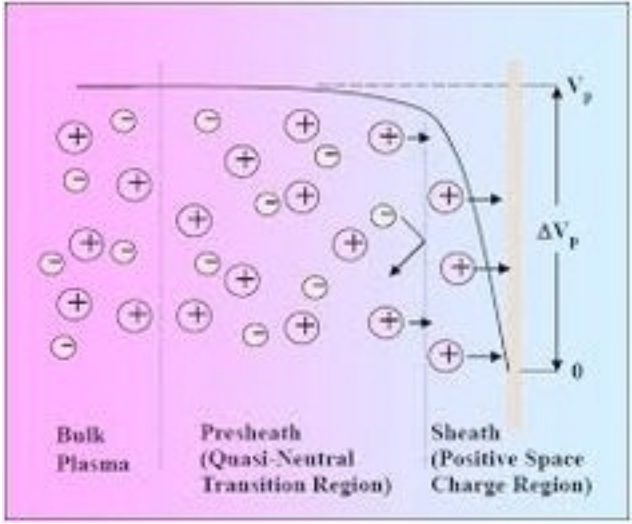
Breakdown voltage
Pasheschen minimum



P pressure
d distance between electrodes

DC plasma


cathode
anode
cathode
Plasma potential
Plasma
negative glow
Ionization rate
Mean electrons energy
X
0
Dark space
D


V_p
ΔV_p
0
Bulk
Plasma
Presheath
(Quasi-Neutral
Transition Region)
Sheath
(Positive Space
Charge Region)

Important plasma parameters

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

Plasma oscillation

Assume: n_0 fixed ions (+) & n_0 moving electrons (–)

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

→ electrons move:

$$\begin{aligned} n_+ &= n_0 \\ n_- &= n_0 + n_1(\mathbf{r},t) \quad ; \quad n_1 \ll n_0 \end{aligned}$$

Electron continuity equation:

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

$$n = n_0 + n_1(\mathbf{r},t) \quad ; \mathbf{u} = \cancelto{0}{\mathbf{u}_0} + \mathbf{u}_1(\mathbf{r},t)$$

($\mathbf{u}_0 = 0$ ↔ electrons are assumed cold)

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

2nd order

Linearized continuity equation (1st order terms only):

$$\frac{\partial n_1}{\partial t} + n_0 \nabla \cdot \mathbf{u}_1 = 0 \quad !!$$

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

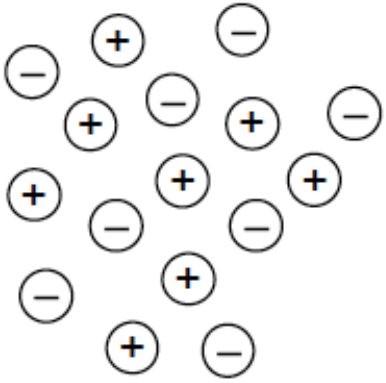
1st Maxwell: $\nabla \cdot \mathbf{E}_1 = -e n_1 / \epsilon_0$

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

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

plasma frequency

Debye screening



Coulomb potential of each charge: $\varphi = \frac{q}{4\pi\epsilon_0 r}$

Assume thermal equilibrium (Boltzmann distribution)

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

α labels the particle populations (e.g., e, p)

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

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

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

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Collisions

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

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

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n = density of atoms (and ions)

Total collistion cross section:

$\sigma_{total} = \sigma_{exitation} + \sigma_{ion} + \sigma_{attachment} + \sigma_{other}$

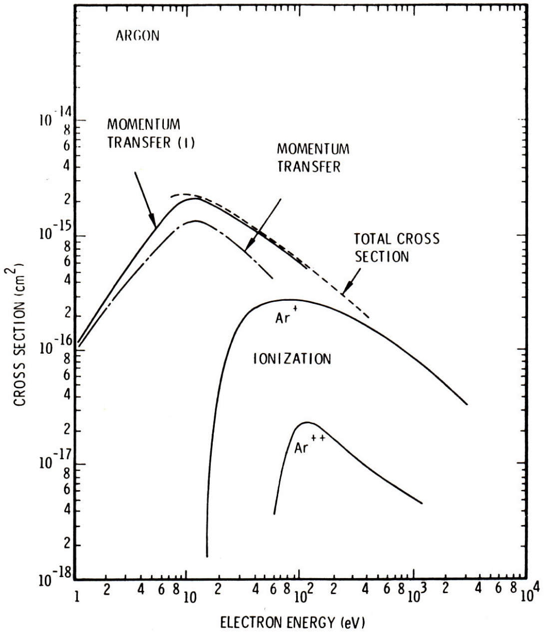
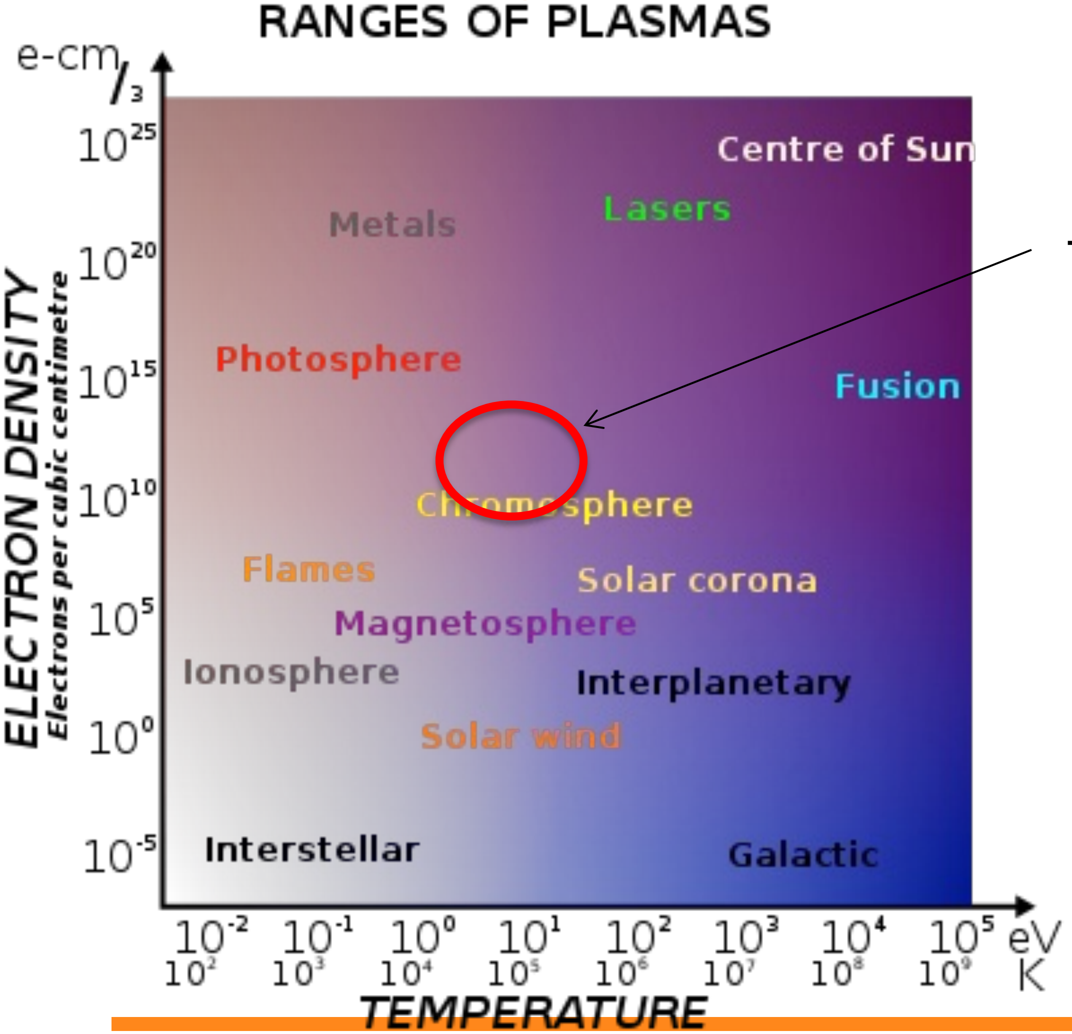


Figure 2.1. Collision cross sections for electrons in Ar gas (from Ref. 1).

Bunshah, Handbook of Deposition Technologies for Films and Coatings Noyes

Different types of plasmas



Thin film plasma processes

Wikipedia

Electron temperature

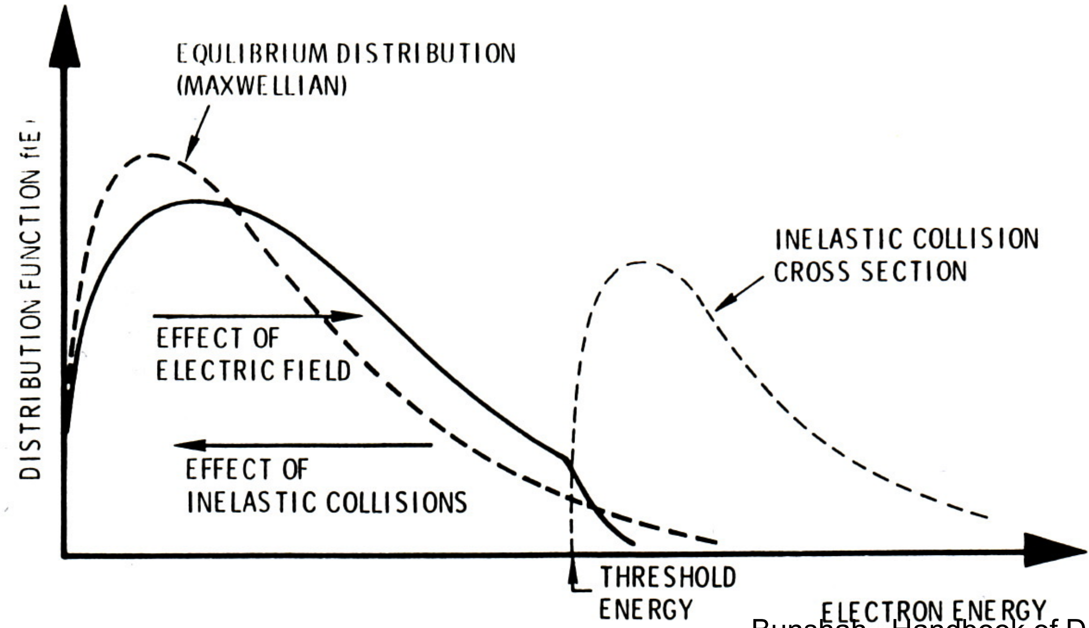


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Figure 2.4. Schematic illustration of electron energy distribution function and inelastic collision cross section.

Electron and ion temperature

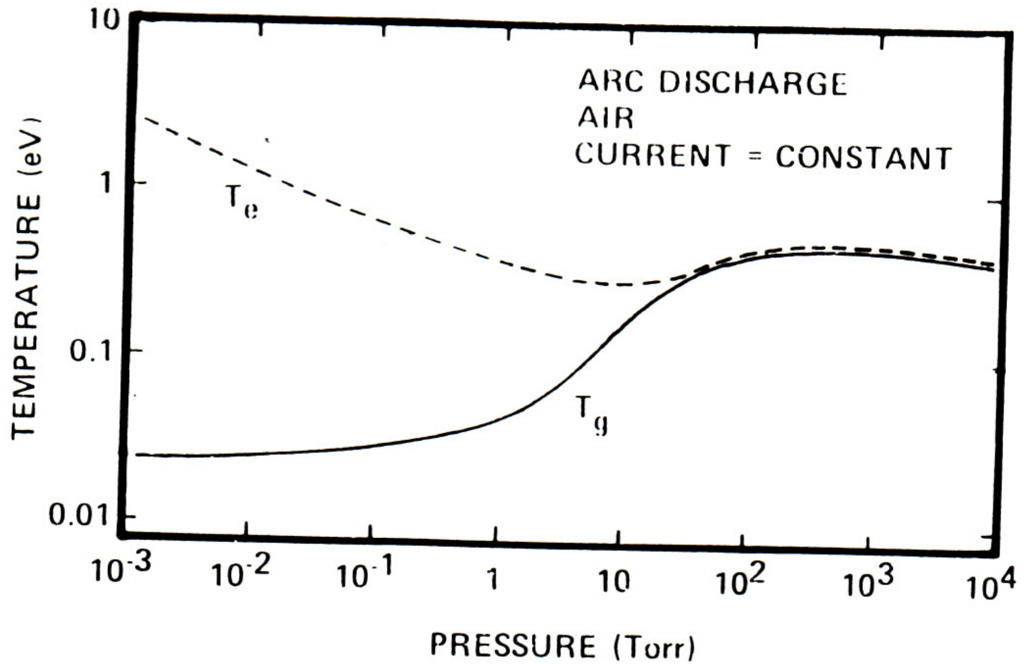

Figure 2.3. Electron (T_e) and gas temperatures (T_g) in an air arc as a function of pressure (from Ref. 5).

Bunshah, Handbook of Deposition Technologies for Films and Coatings Noyes

Plasma sheath

Sheath thickness $d_s \sim$ constant* λ_D

constant ≈ 5 – 40

Glow discharge $d_s \approx 0.15 – 2$ mm

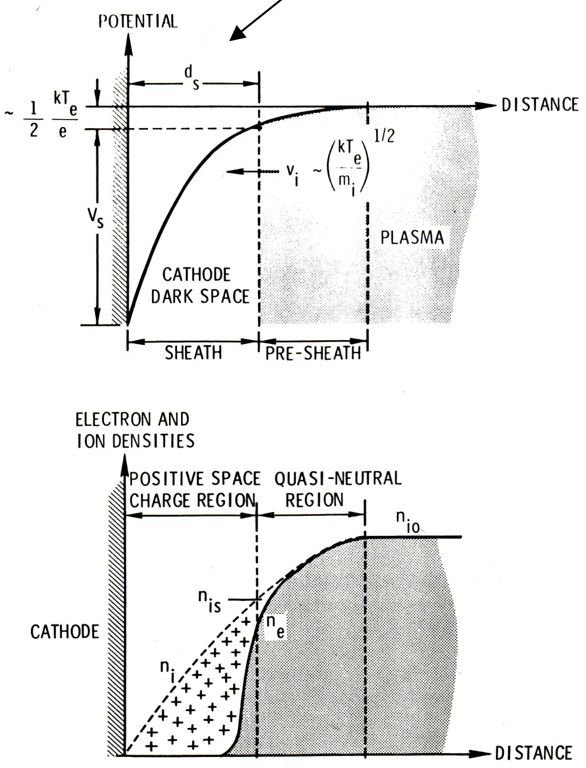

Figure 2.9. Schematic representation of the positive space-charge sheath that develops over a cathode (from Ref. 1).

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Cold cathode discharge

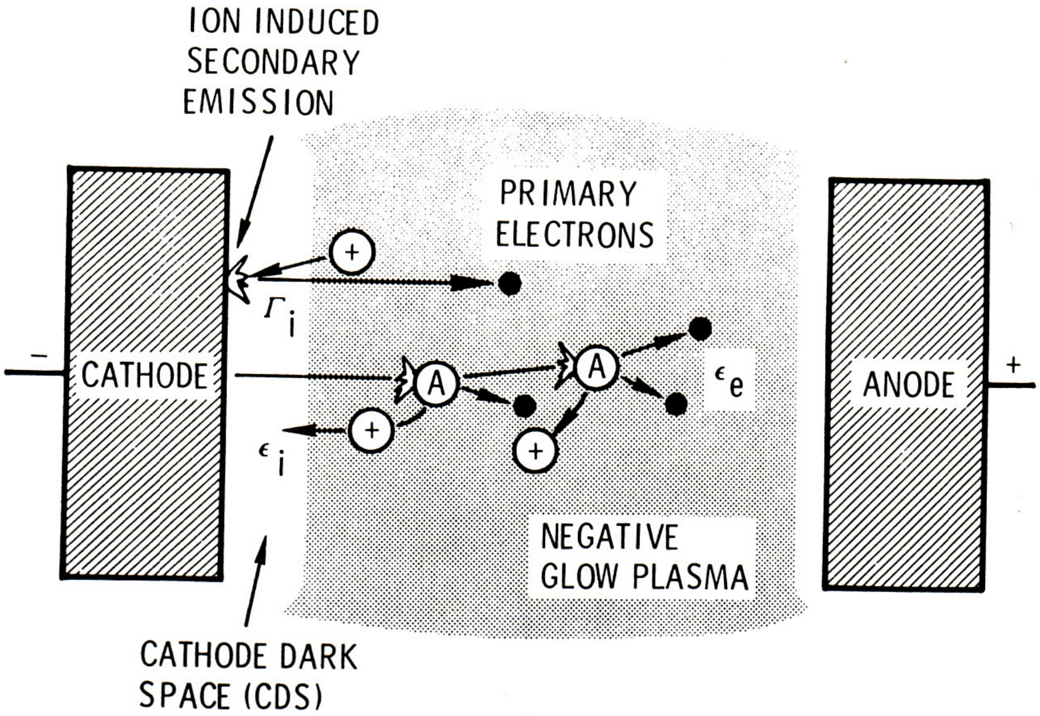

Figure 2.18. Schematic illustration of a cold-cathode discharge.

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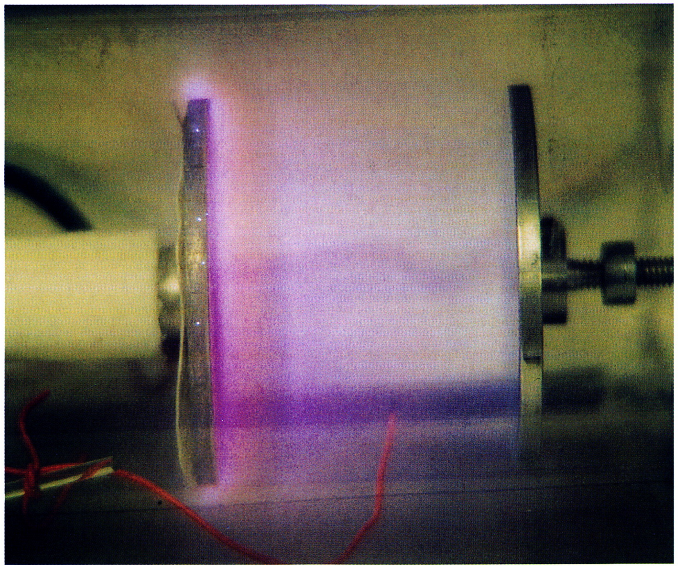
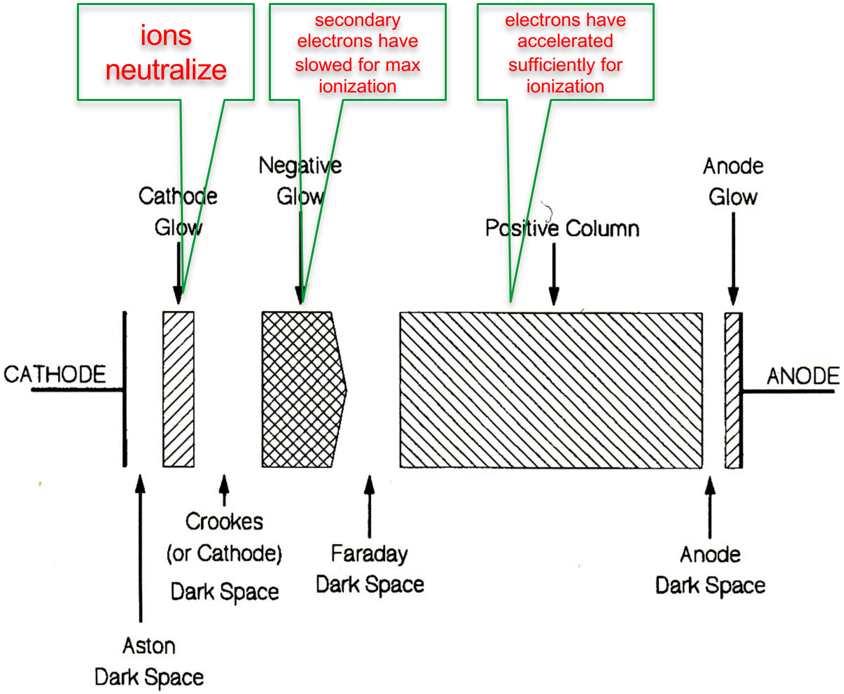
Luminous regions in DC plasma



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/cm².



ions neutralize

secondary electrons have slowed for max ionization

electrons have accelerated sufficiently for ionization

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].

Mahan, Physical Vapor Deposition of Thin Films, Wiley

Practical sputtering plasma -1

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

Practical sputtering plasma -2

- VDC 1000V
- Vp 8V
- Current density at cathode 2 mA/cm^2
- Cathode sheath L 2 mm
- mean free path λ 50 μm

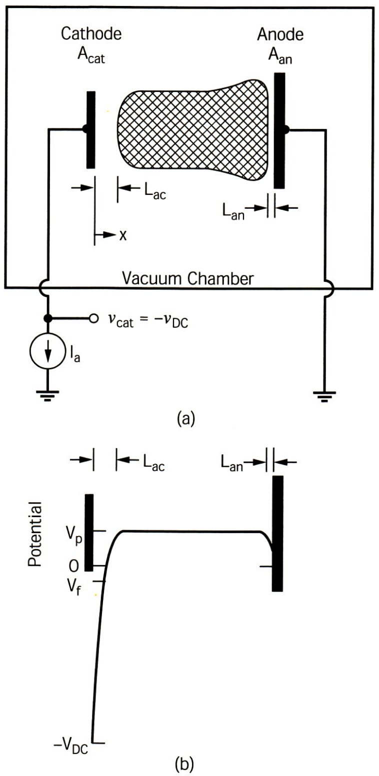


Figure VI.8 (*a*) Schematic diagram of a DC sputtering discharge; (*b*) the potential profile (not to scale, as $V_p - V_f$ is typically much less than V_{DC}).

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Circuit models of DC plasma discharge

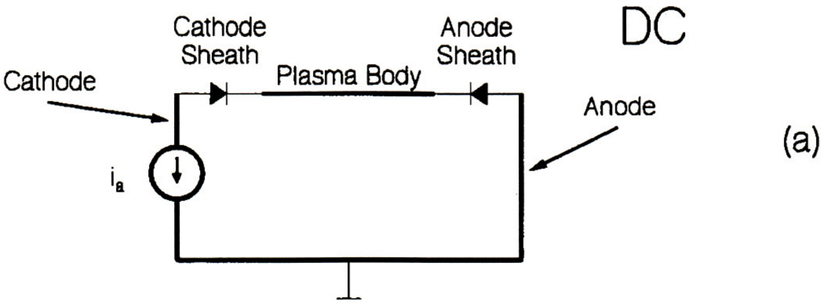

Figure VI.9 Circuit models for (*a*) a DC sputtering discharge and (*b*) a capacitive RF sputtering discharge.

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Ion energy at cathode

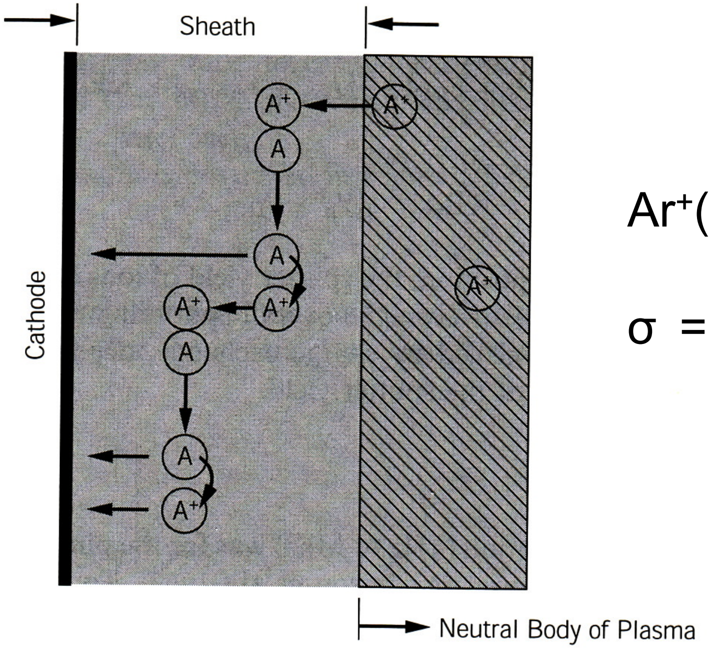

Figure VI.10 The process of symmetric charge exchange within the cathode sheath. When two charge exchange events occur, as shown here, a single ion entering the sheath is converted into two neutrals plus an ion, all of which strike the cathode (but with kinetic energies corresponding to only a fraction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

$\mathrm{Ar^+(hot) + Ar(cold)} \rightarrow \mathrm{Ar(hot)+Ar^+(cold)}$

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

Mahan, Physical Vapor Deposition of Thin Films, Wiley

AC plasma methods

AC plasma

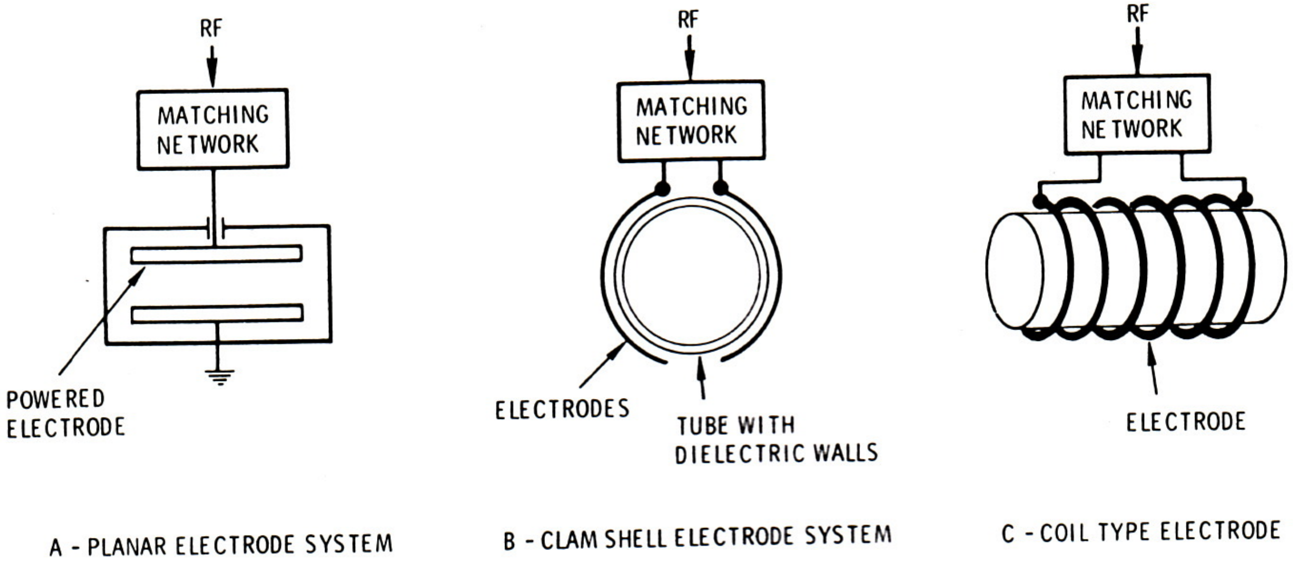

Figure 2.12. Schematic illustration of glow discharge devices commonly used in plasma-assisted materials processing.

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Forming of self-bias in AC discharge

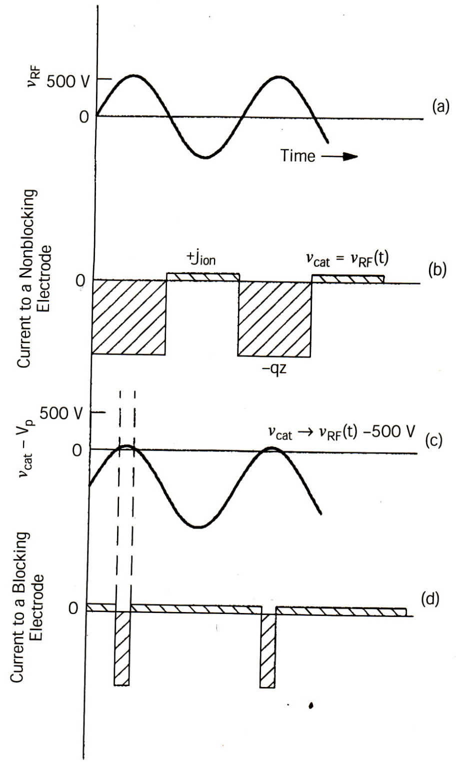

Figure VI.11 DC self-bias. Potentials and currents for RF excitation of (*a*–*b*) nonblocking and (*c*–*d*) blocking electrodes.

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)

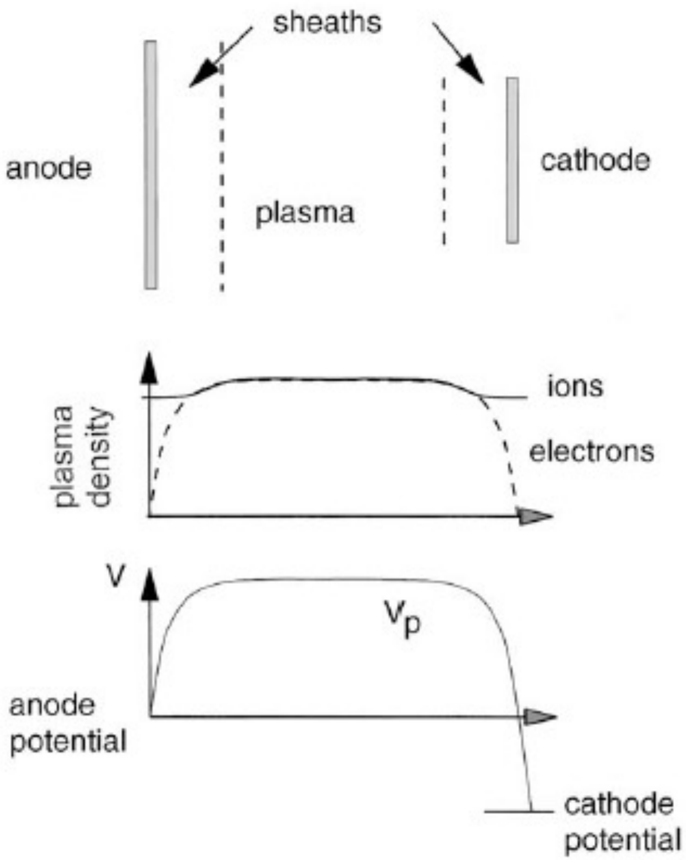

Fig. 7. Electron and ion distributions which create sheaths between the neutral plasma and the walls.

Circuit models of RF plasma discharge

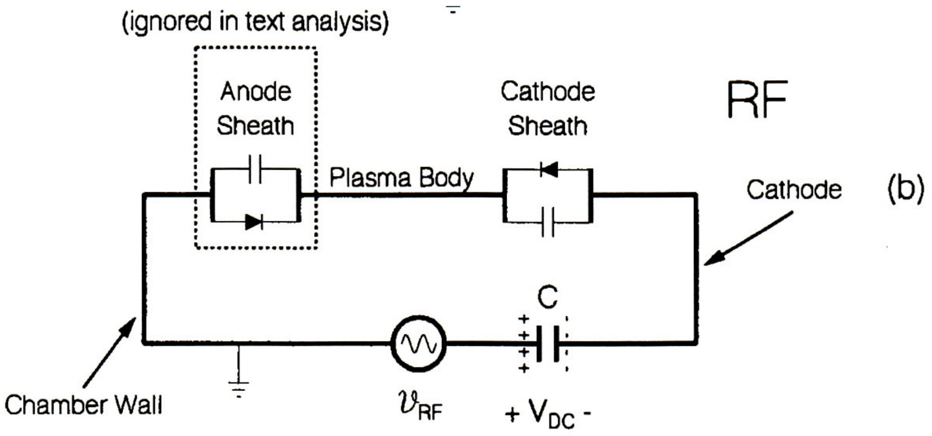

Figure VI.9 Circuit models for (*a*) a DC sputtering discharge and (*b*) a capacitive RF sputtering discharge.

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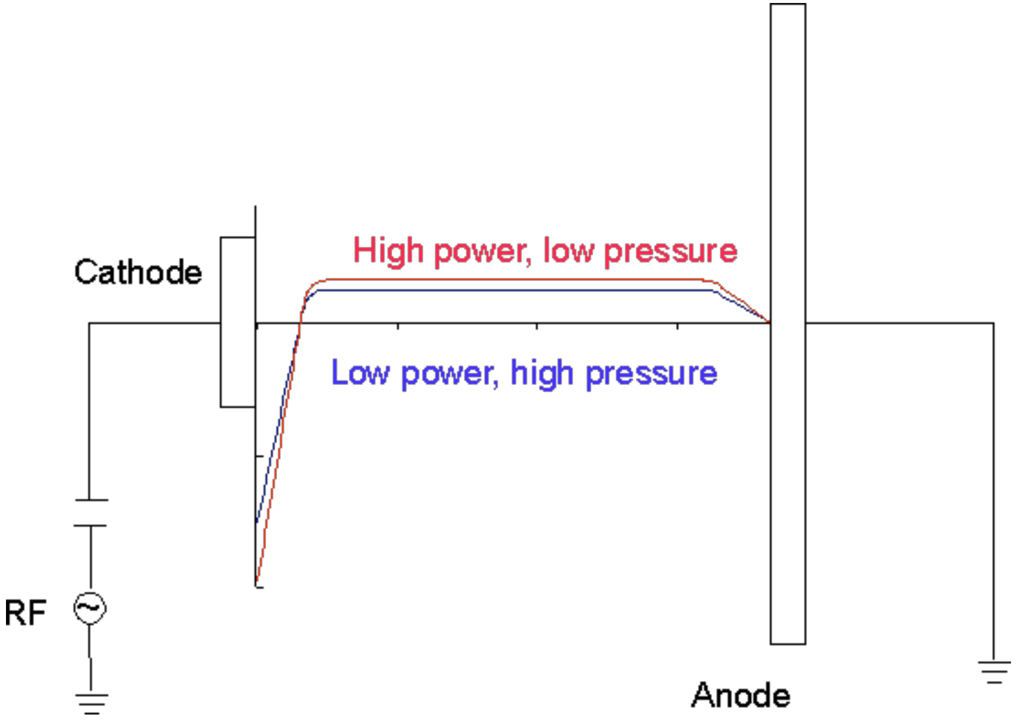
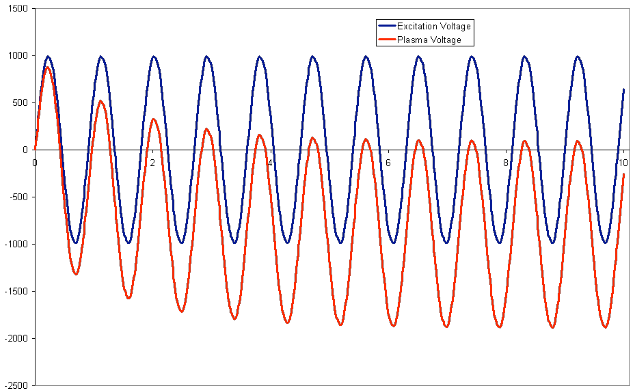
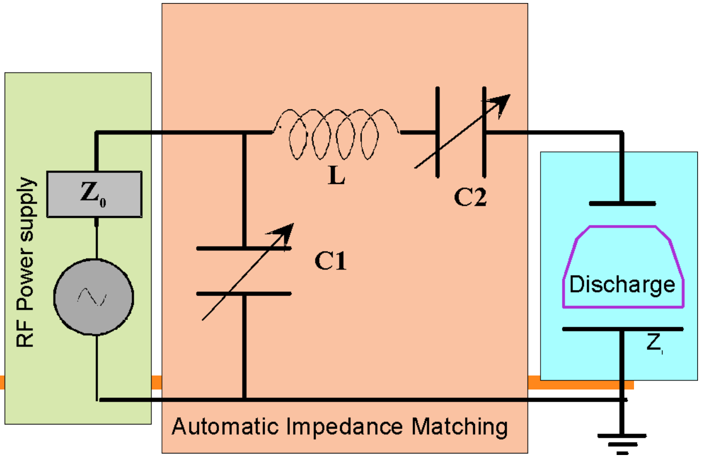
RF Plasma glow discharge



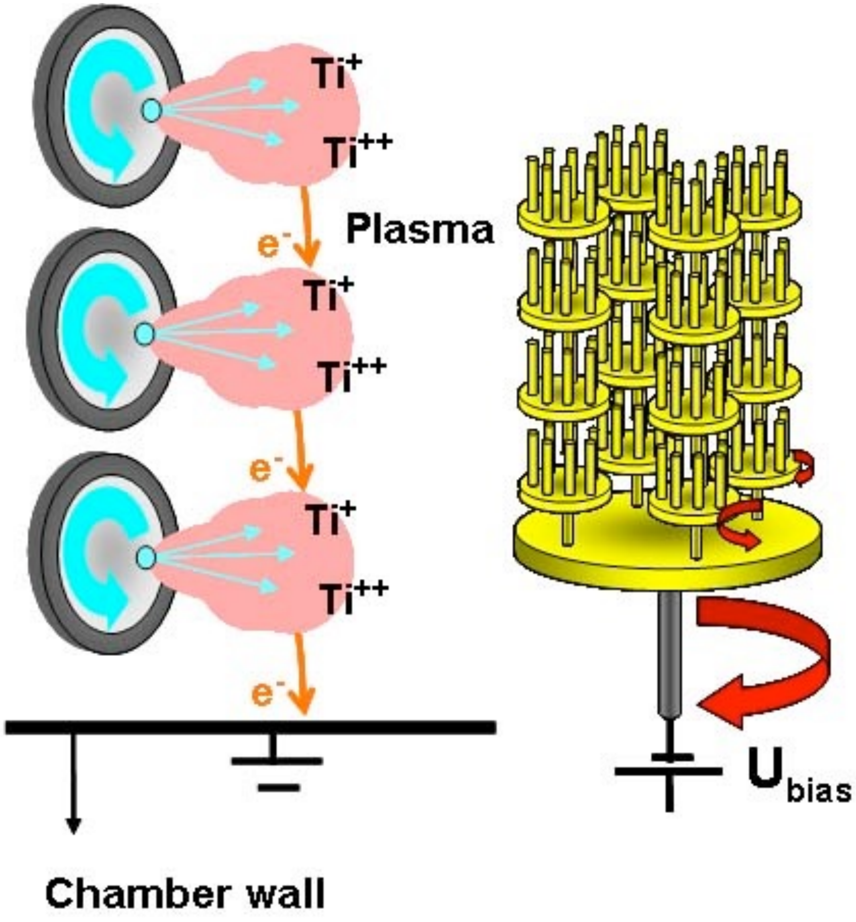




http://www.spectruma.de

Arc plasma

Arc discharge deposition



Arc discharge video

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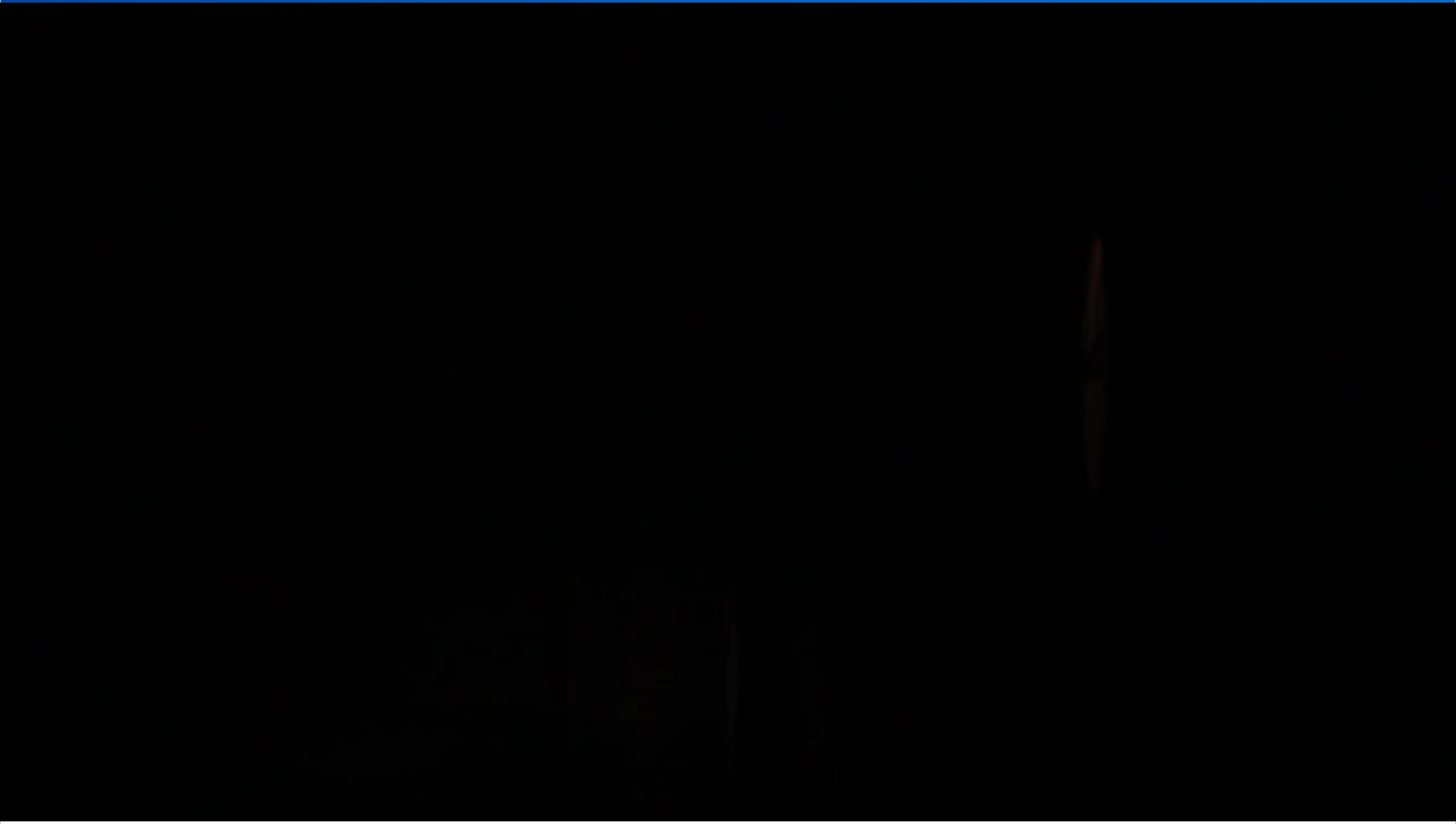
Particles in cathodic arc



https://www.youtube.com/watch?v=gM86v350HhM&t=60s

Cathodic arc spot evolution

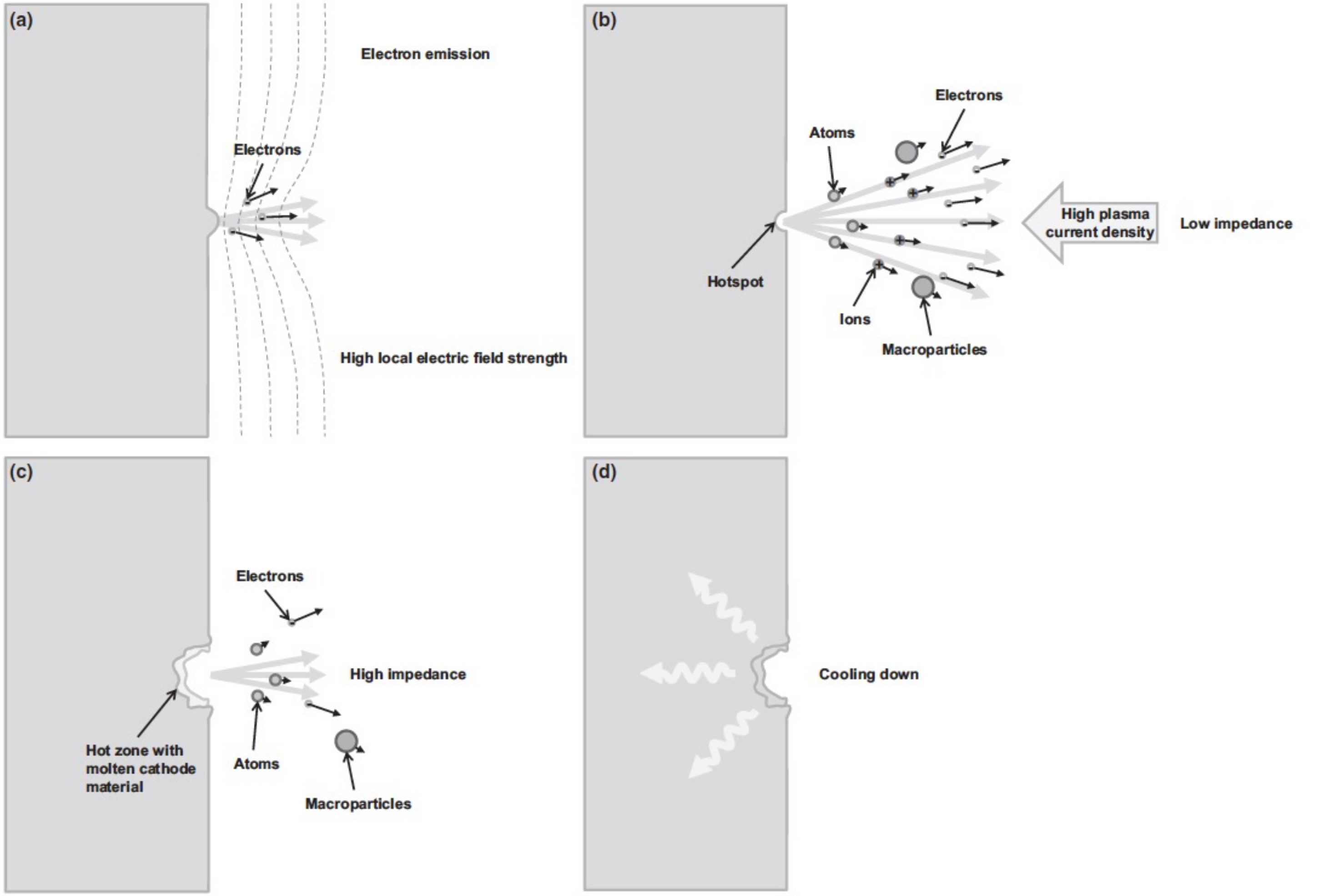
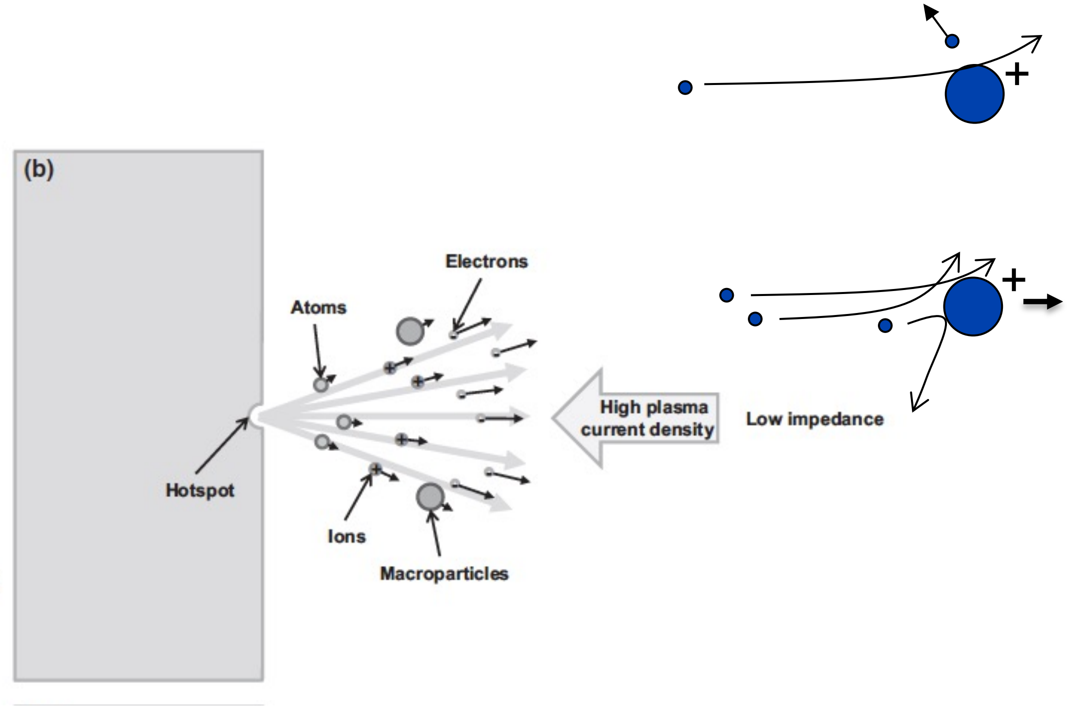


Figure 13 The evolution of the cathode spot in four stages. (a) Pre-explosion; (b) explosive stage; (c) cooling with molten cathode material; and (d) final cooling.

Koskinen, J. Cathodic-Arc and Thermal-Evaporation Deposition. In Comprehensive Materials Processing;Cameron, D., Ed.; Vol. 4; Elsevier Ltd., 2014, 2014; pp 3–55. ISBN: 9780080965321

Electron wind causes ionization and acceleration of atoms



Ionization of atoms

Acceleration of ions

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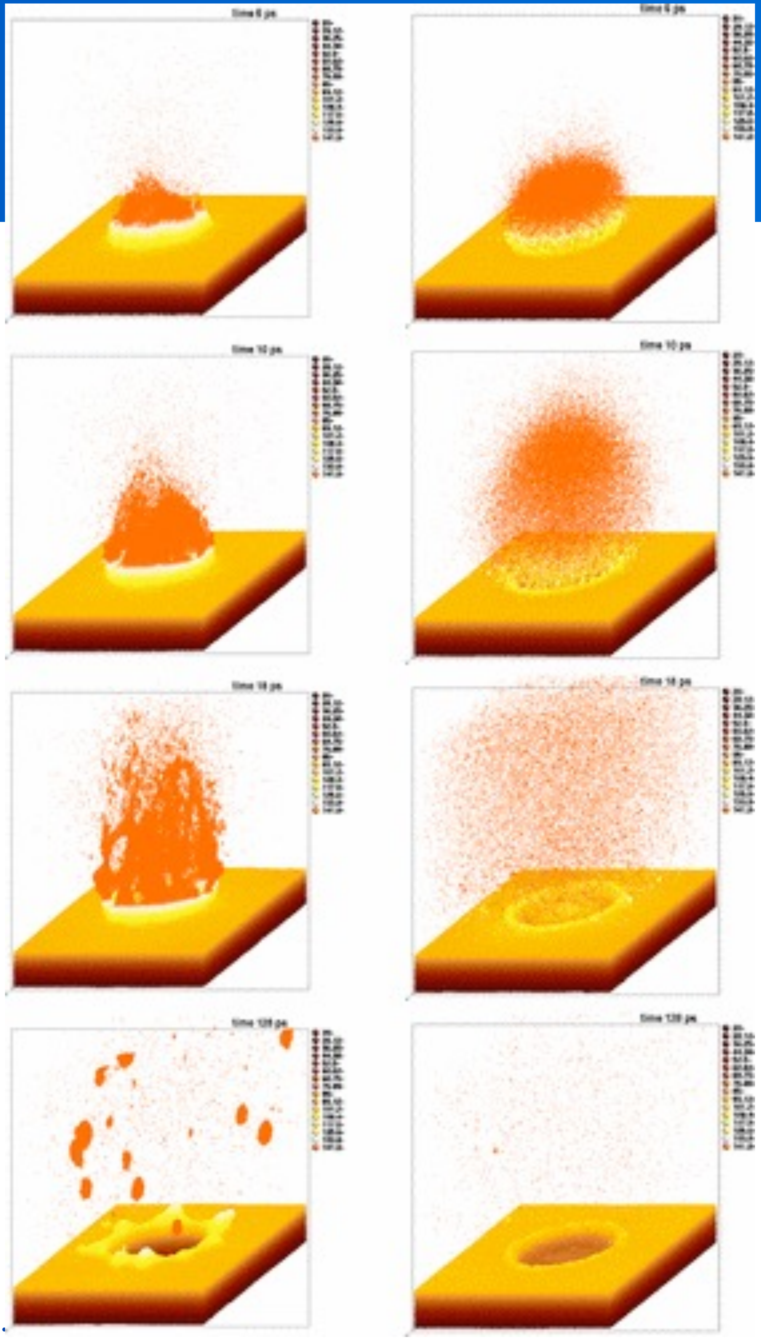
Arc spot evolution by numeric simulation



Left: energetic plasma ion flux

Right: local thermal heating

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Cu atoms, Cu+ ions and electrons near cathode spot by numerical simulations

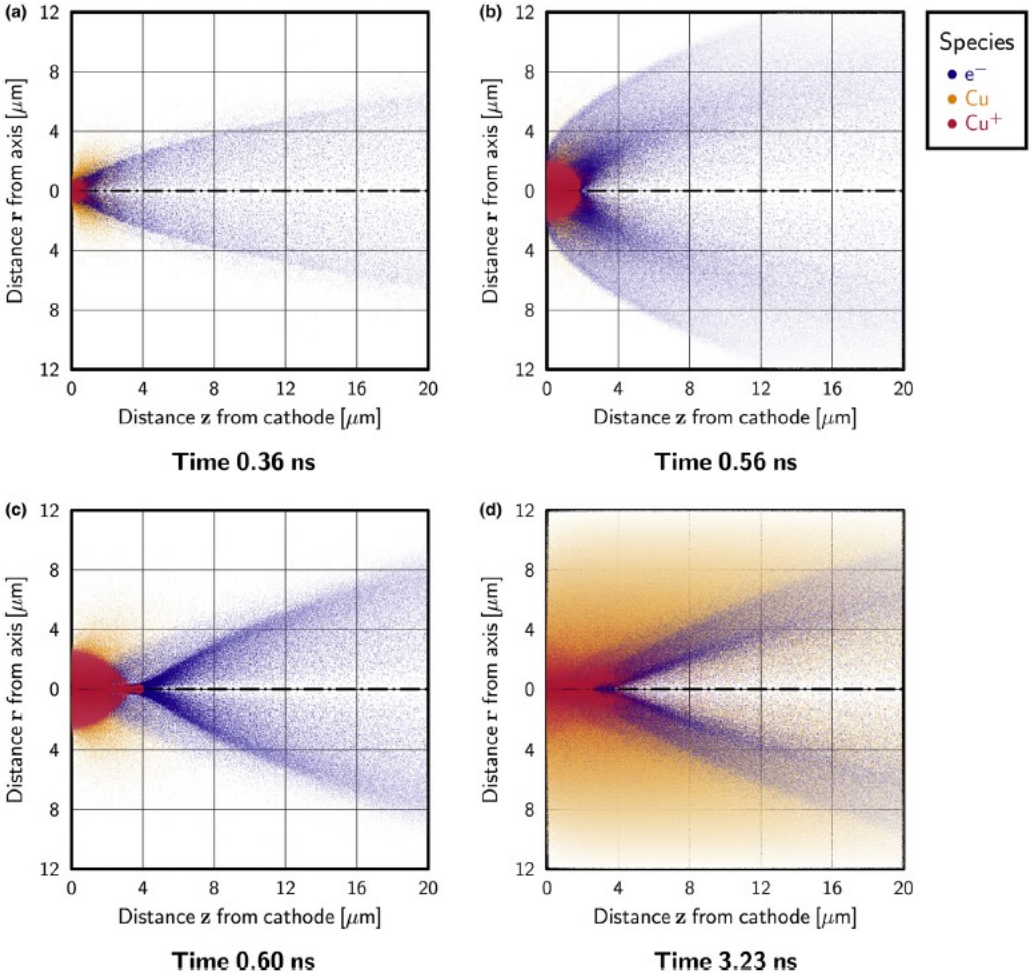
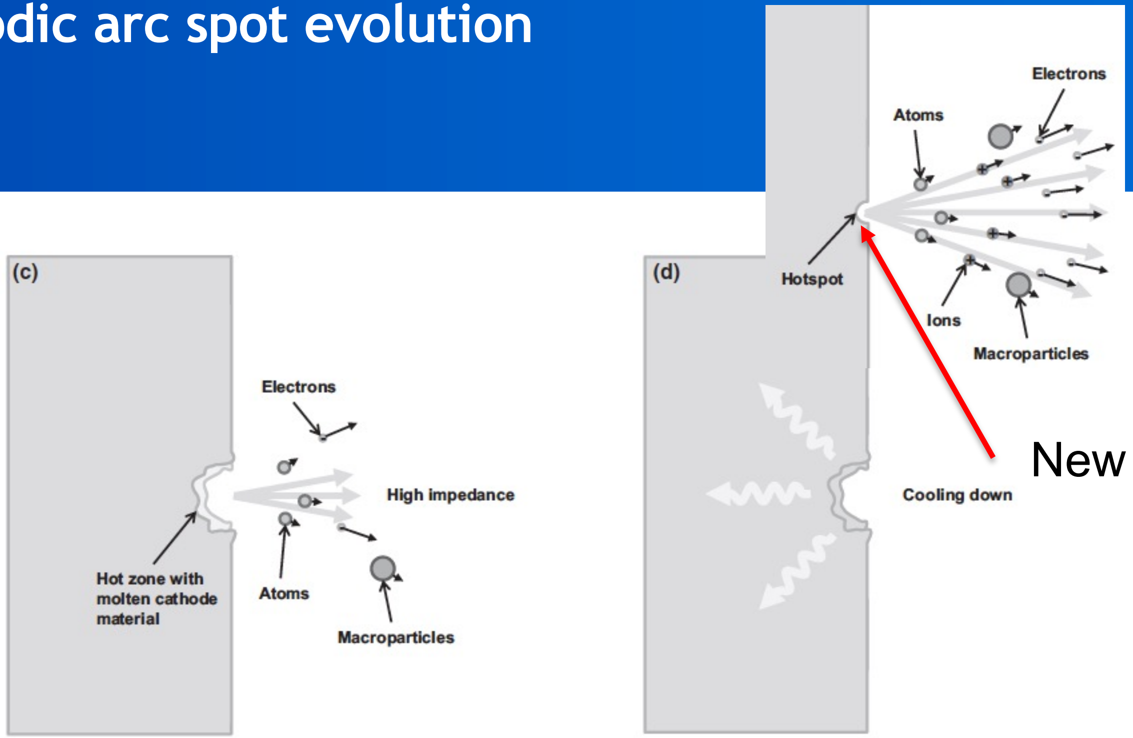


Figure 14 Time evolution of the plasma initiation process in four time steps obtained by numerical modeling. Reproduced from Timko, H. Modelling Vacuum Arcs: From Plasma Initiation to Surface Interactions. Report Series in Physics HU-P-D188, Theses, 2011.

Koskinen, J. Cathodic-Arc and Thermal-Evaporation Deposition. In Comprehensive Materials Processing;Cameron, D., Ed.; Vol. 4; Elsevier Ltd., 2014, 2014; pp 3–55. ISBN: 9780080965321

Cathodic arc spot evolution

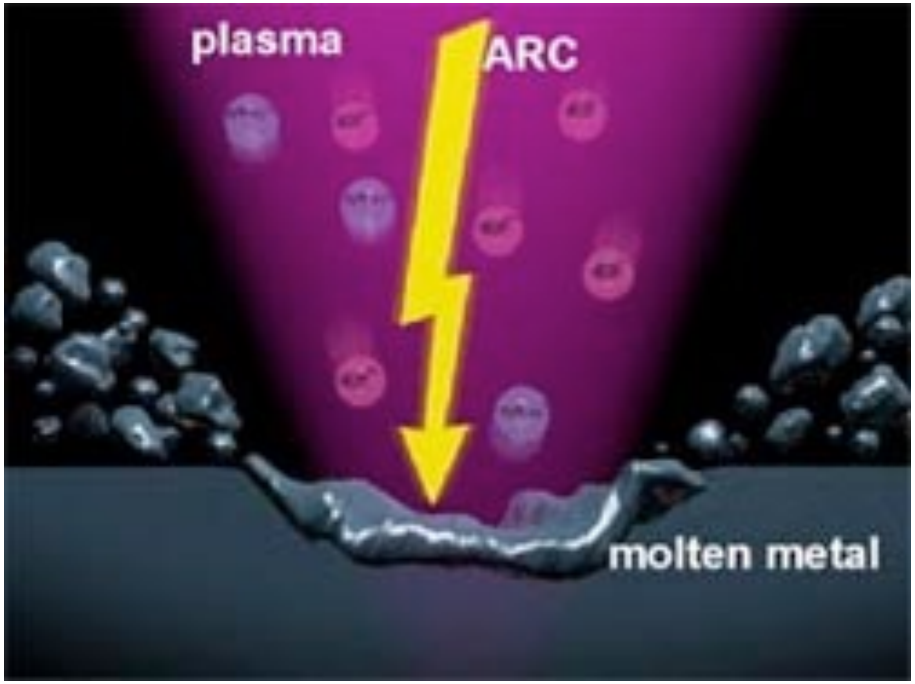


New hot cathodis spot

Figure 13 The evolution of the cathode spot in four stages. (a) Pre-explosion; (b) explosive stage; (c) cooling with molten cathode material; and (d) final cooling.

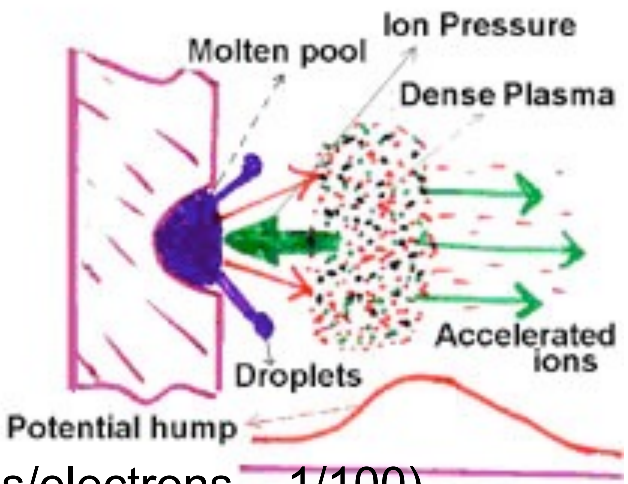
Koskinen, J. Cathodic-Arc and Thermal-Evaporation Deposition. In Comprehensive Materials Processing;Cameron, D., Ed.; Vol. 4; Elsevier Ltd., 2014, 2014; pp 3–55. ISBN: 9780080965321

Arc disharge – cathode spot



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
- $10^6 - 10^8$ 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
- electons 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 µm diam.I are formed

Timko, Nordlund simulations
http://prb.aps.org/supplemental/PRB/v81/i18/e184109

Filtered arc

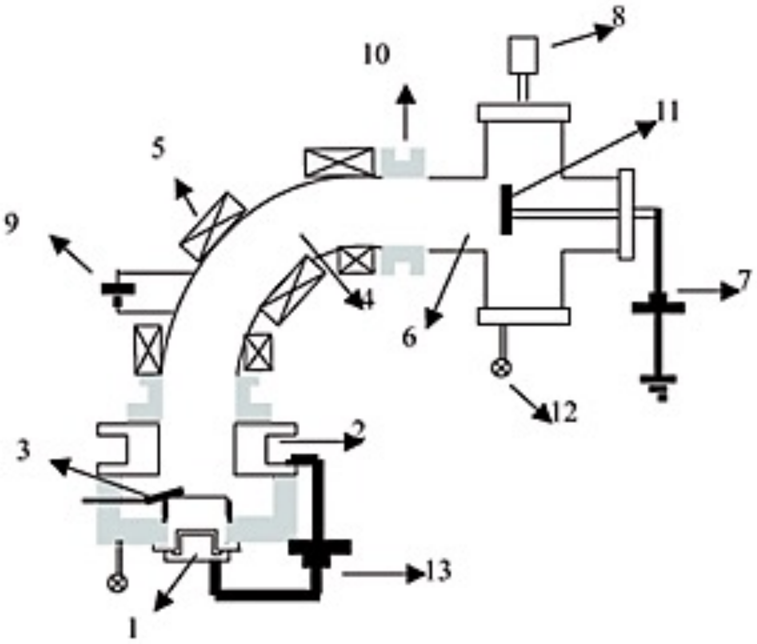
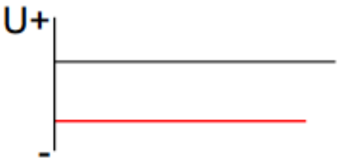


Figure 1. Scheme of the DCF2 device. (1) cathode; (2) anode; (3) trigger; (4) quarter torus magnetic filter; (5) torus coil; (6) deposition chamber; (7) probe bias source; (8) diagnostic port; (9) filter bias source; (10) insulators; (11) collecting probe; (12) vacuum pumping systems; (13) arc source.

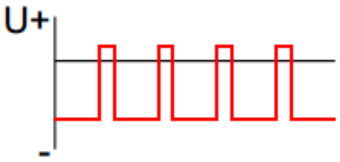
PULSED SPUTTERING

Definitions

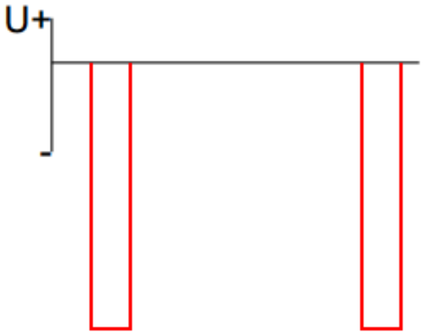
- DC-sputtering



- Pulsed DC



- HiPIMS



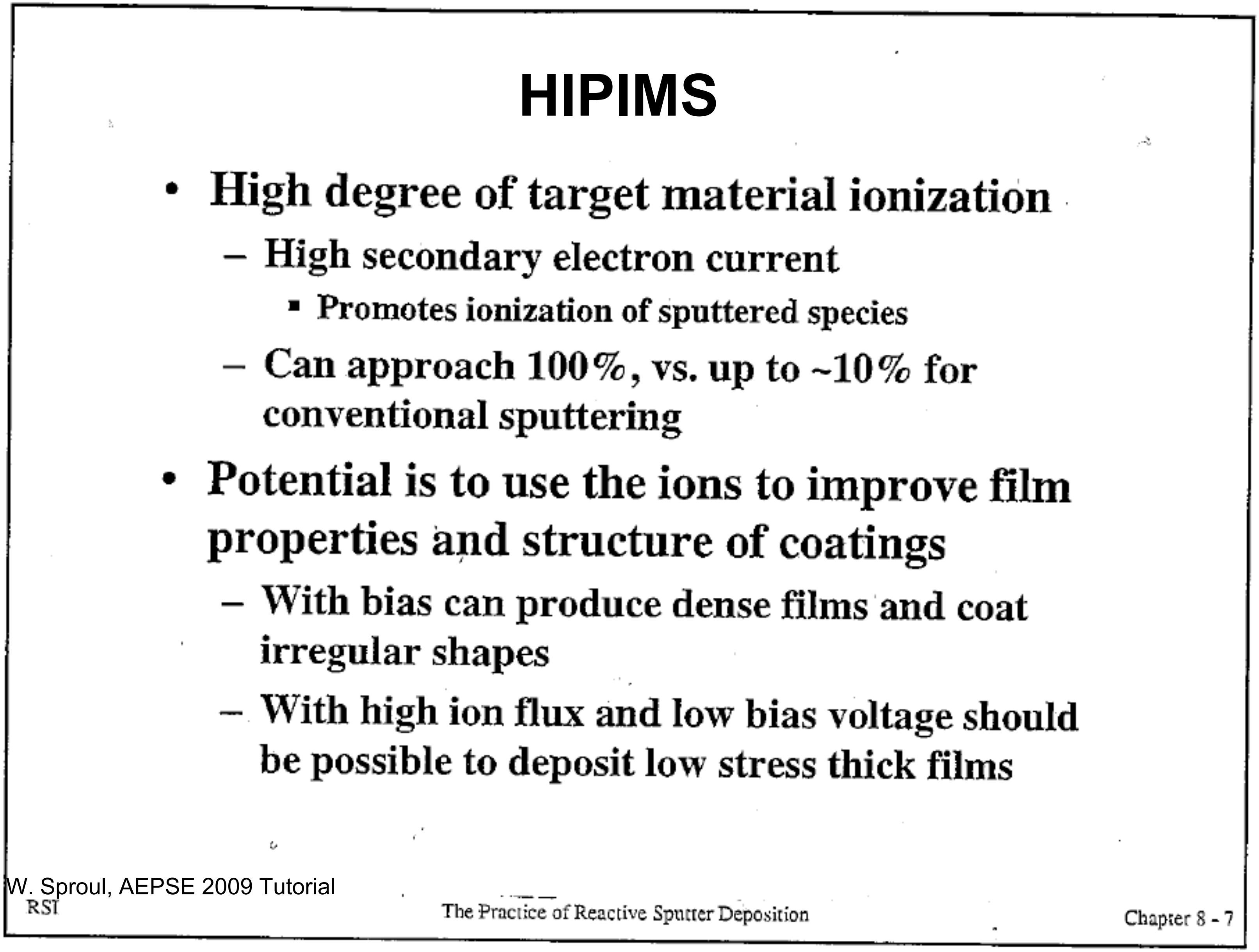
HIPIMS

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/cm²
  - 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 No
Sputter Technique Utilizing Very High Target Power Densities,” Surf. Coat. Tec

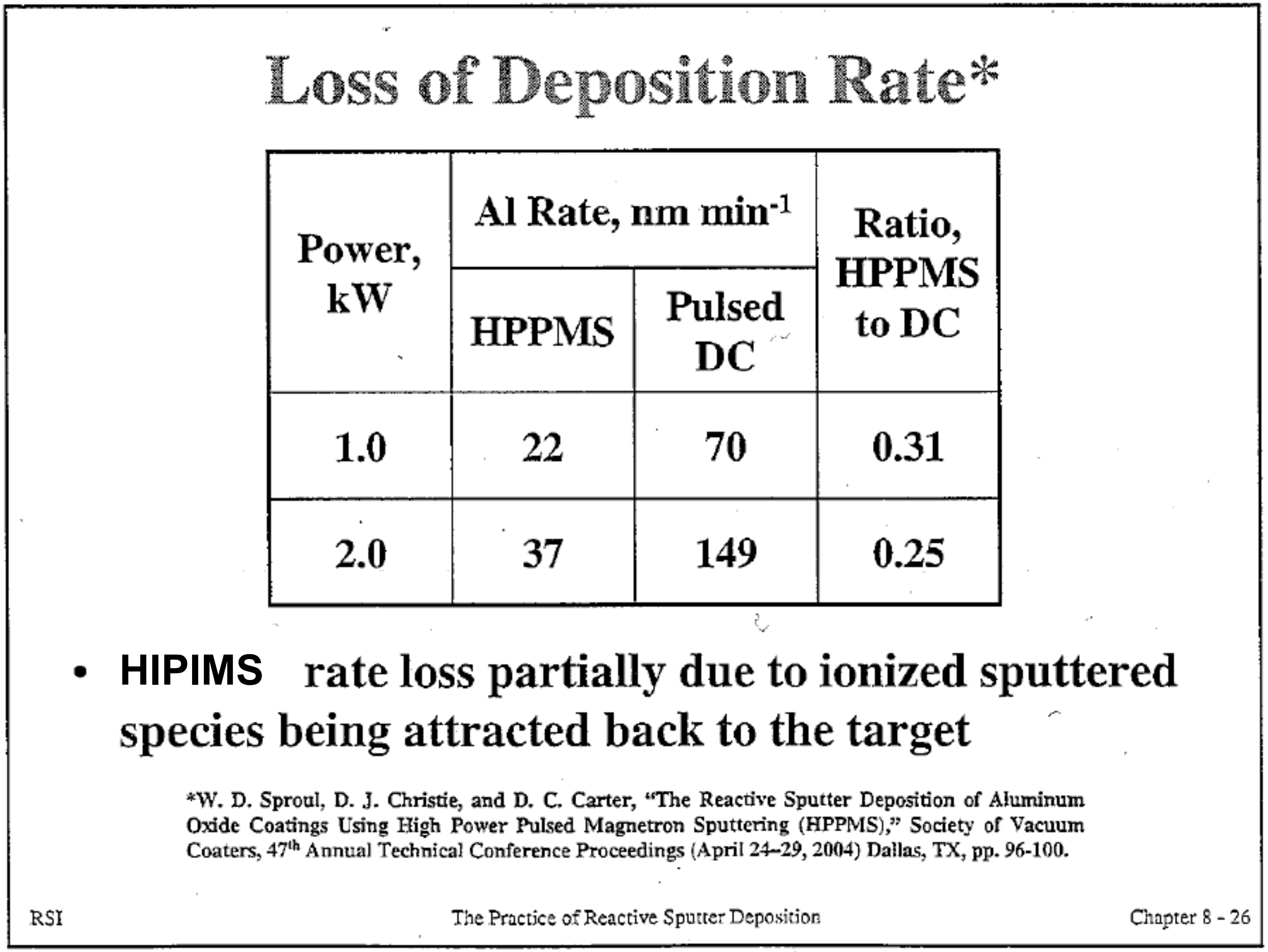
Pulsed Plasma
Diffusion”



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

W. Sproul, AEPSE 2009 Tutorial



Loss of Deposition Rate*

Power, kW	Al Rate, nm min^{-1}		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, 47th Annual Technical Conference Proceedings (April 24-29, 2004) Dallas, TX, pp. 96-100.

W. Sproul, AEPSE 2009 Tutorial

Fluxes of ions in HIPIMS

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

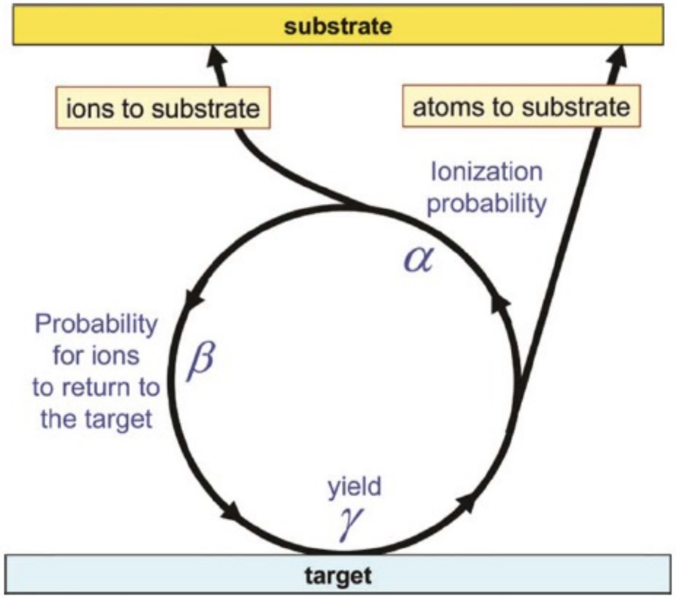
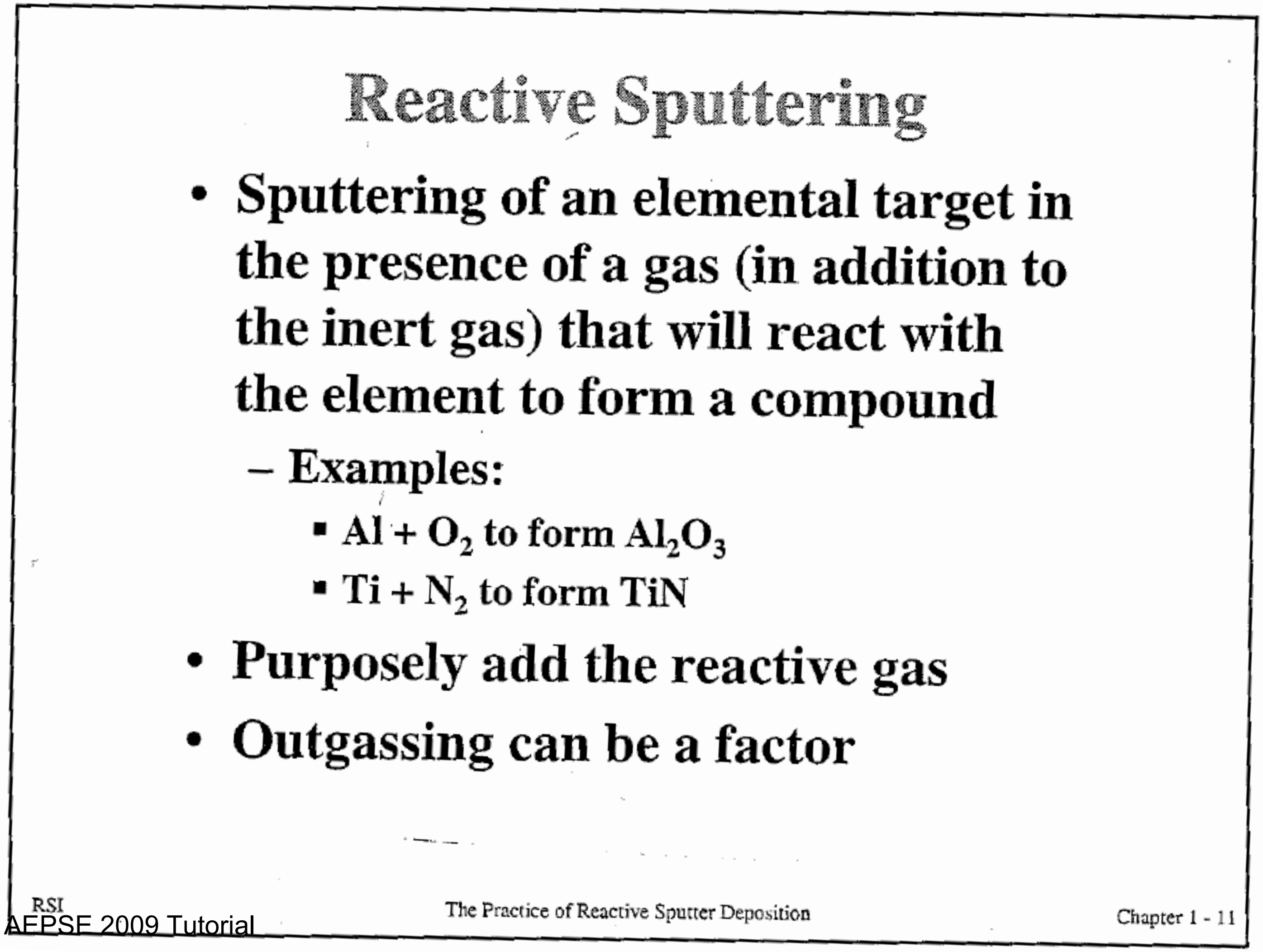


FIG. 2. (Color online) Schematic presentation of the fluxes involved in the deposition by HIPIMS under conditions when the plasma is dominated by metal sputtered from the target; α, β, and γ are the ionization probability, the return probability, and the sputtering yield, respectively; for further explanations 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:
    - Al + O_2 to form Al_2O_3
    - Ti + N_2 to form TiN
- Purposely add the reactive gas
- Outgassing can be a factor

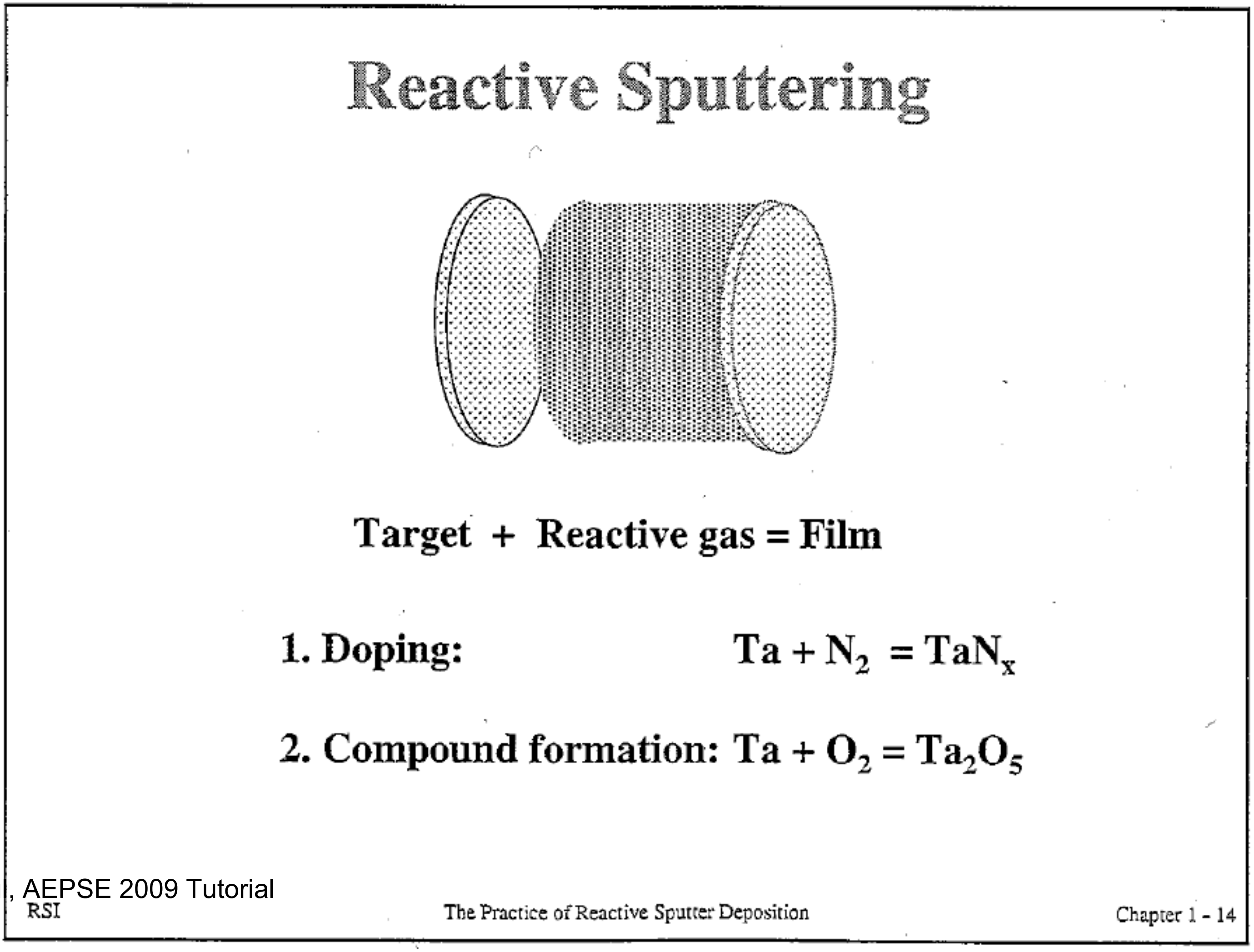
RSI

The Practice of Reactive Sputter Deposition

Chapter 1 - 11

W. Sproul, AEPSF 2009 Tutorial

Reactive sputtering



Reactive Sputtering

Target + Reactive gas = Film

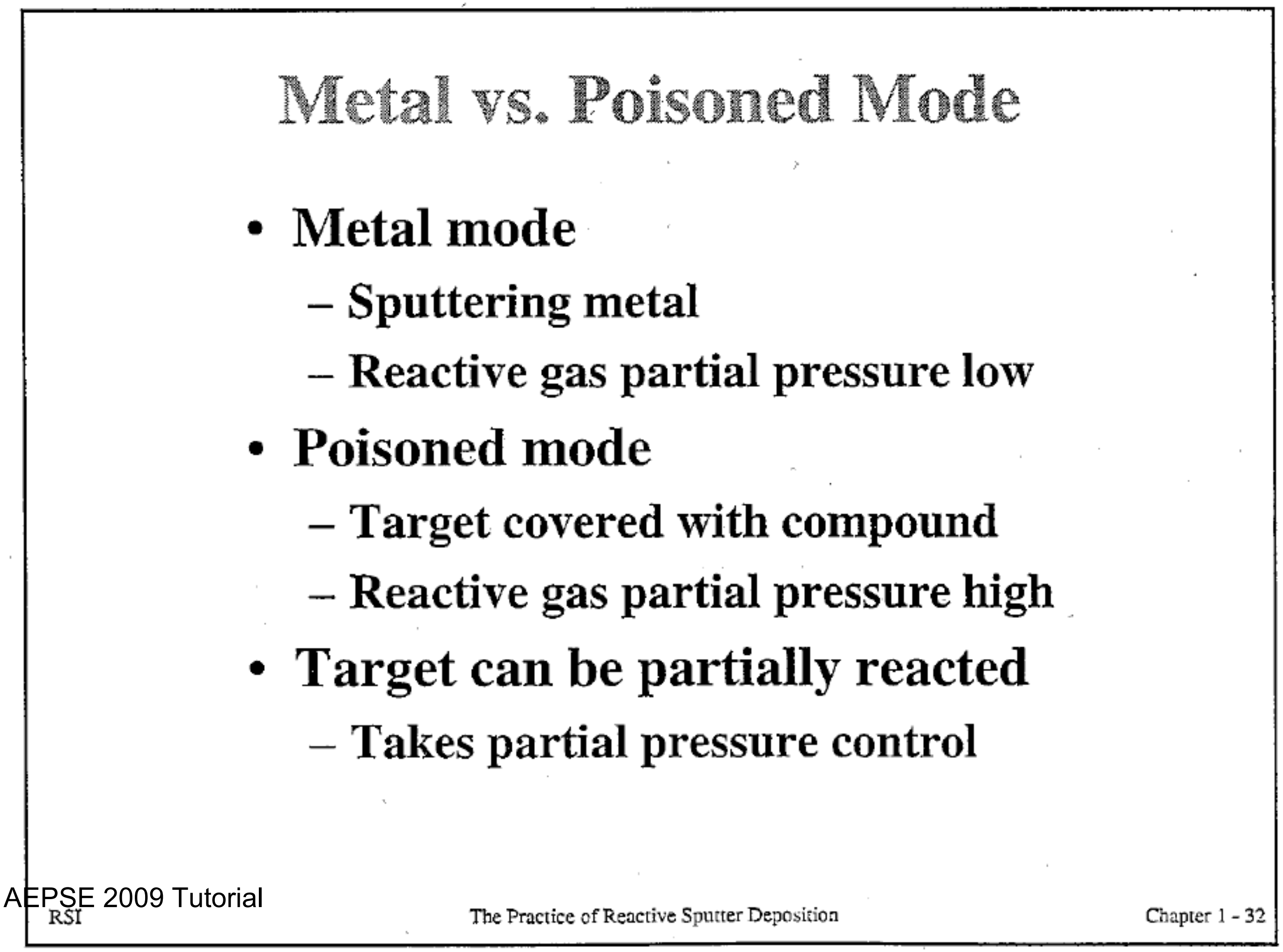
1. Doping: $Ta + N_2 = TaN_x$

2. Compound formation: $Ta + O_2 = Ta_2O_5$

RSI The Practice of Reactive Sputter Deposition Chapter 1 - 14

W. Sproul, AEPSE 2009 Tutorial

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

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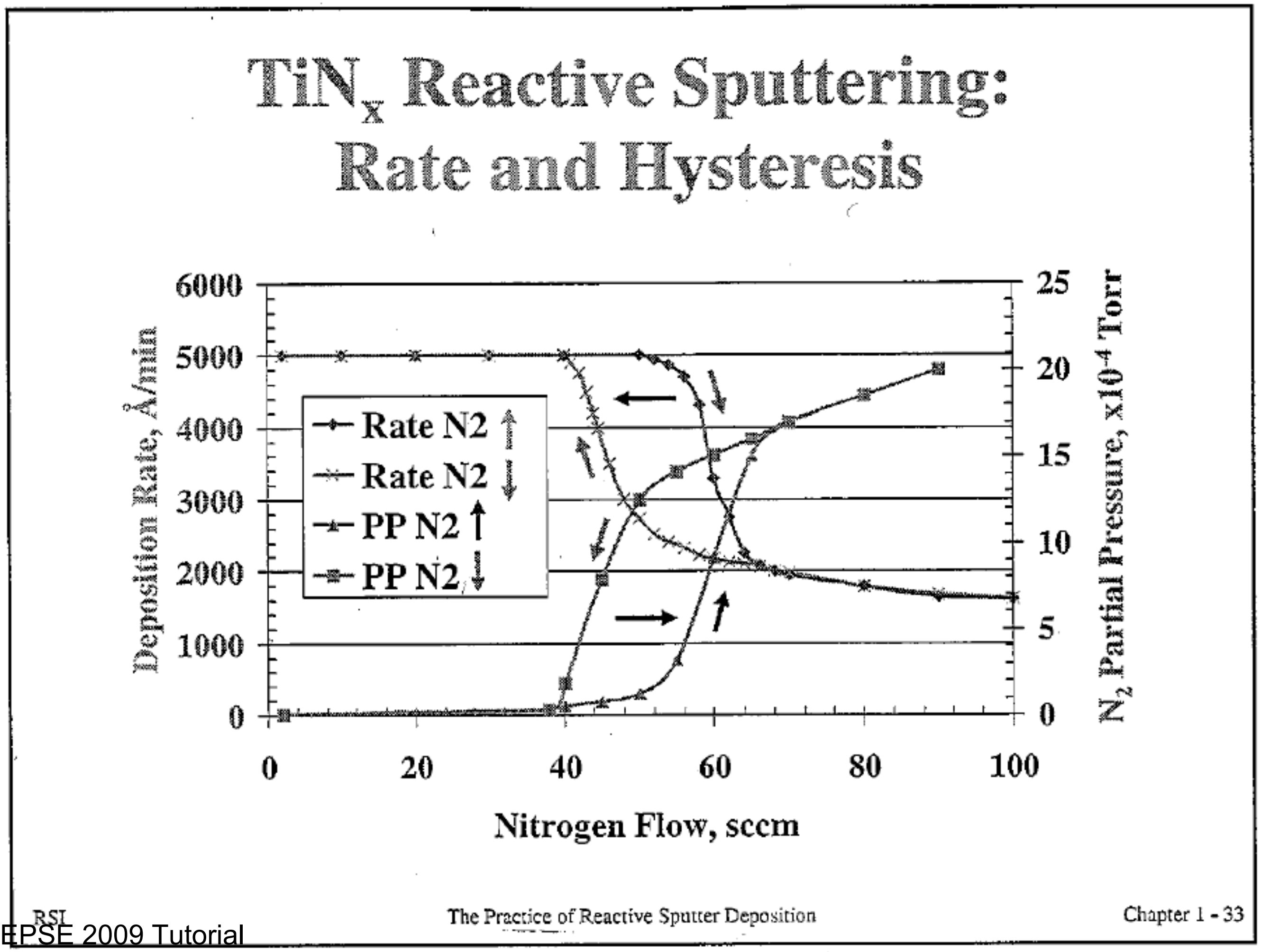
Reactive sputtering



TiN_x Reactive Sputtering: Rate and Hysteresis

RSI

The Practice of Reactive Sputter Deposition

Chapter 1 - 33

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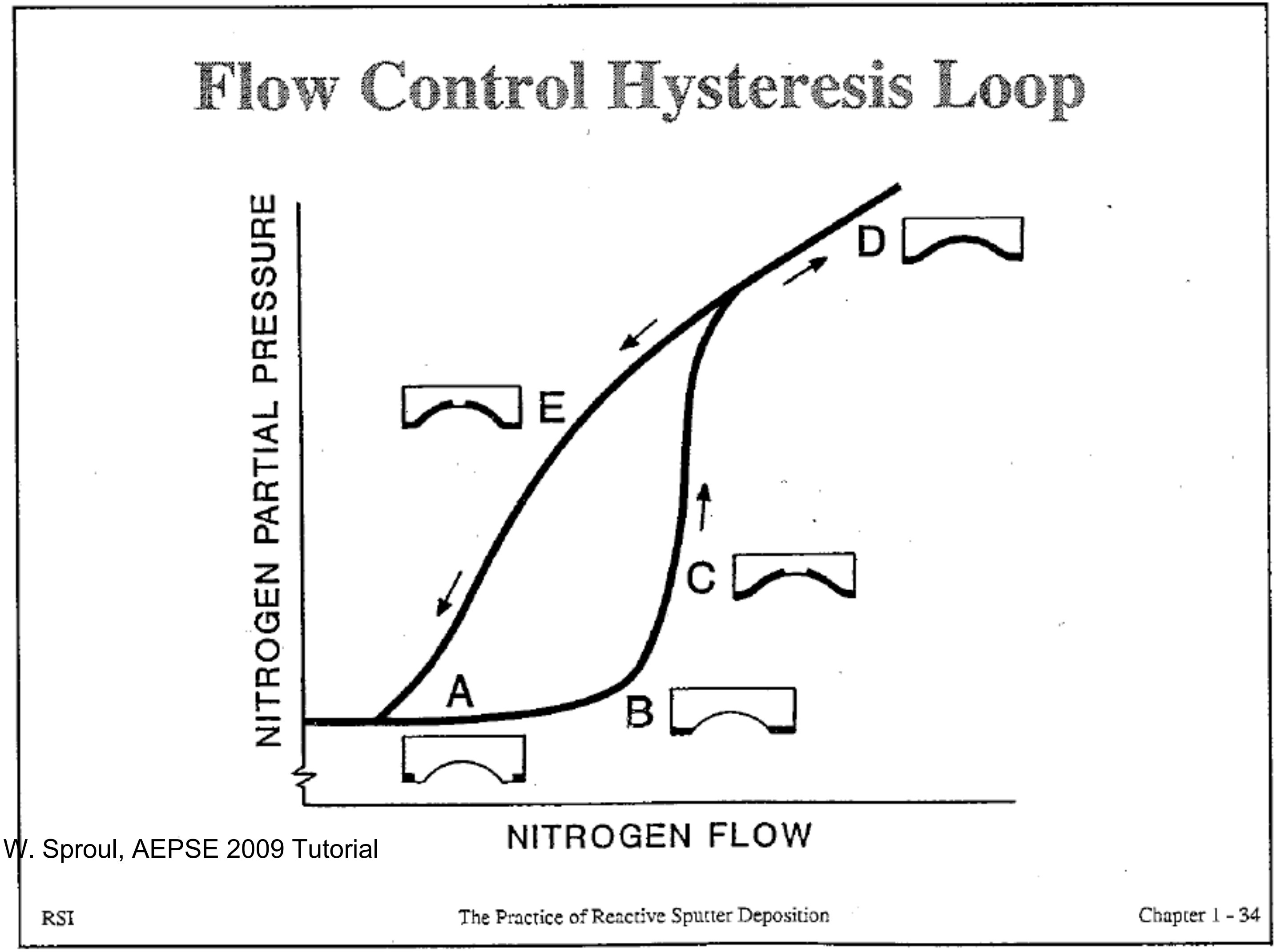
Reactive sputtering



Flow Control Hysteresis Loop

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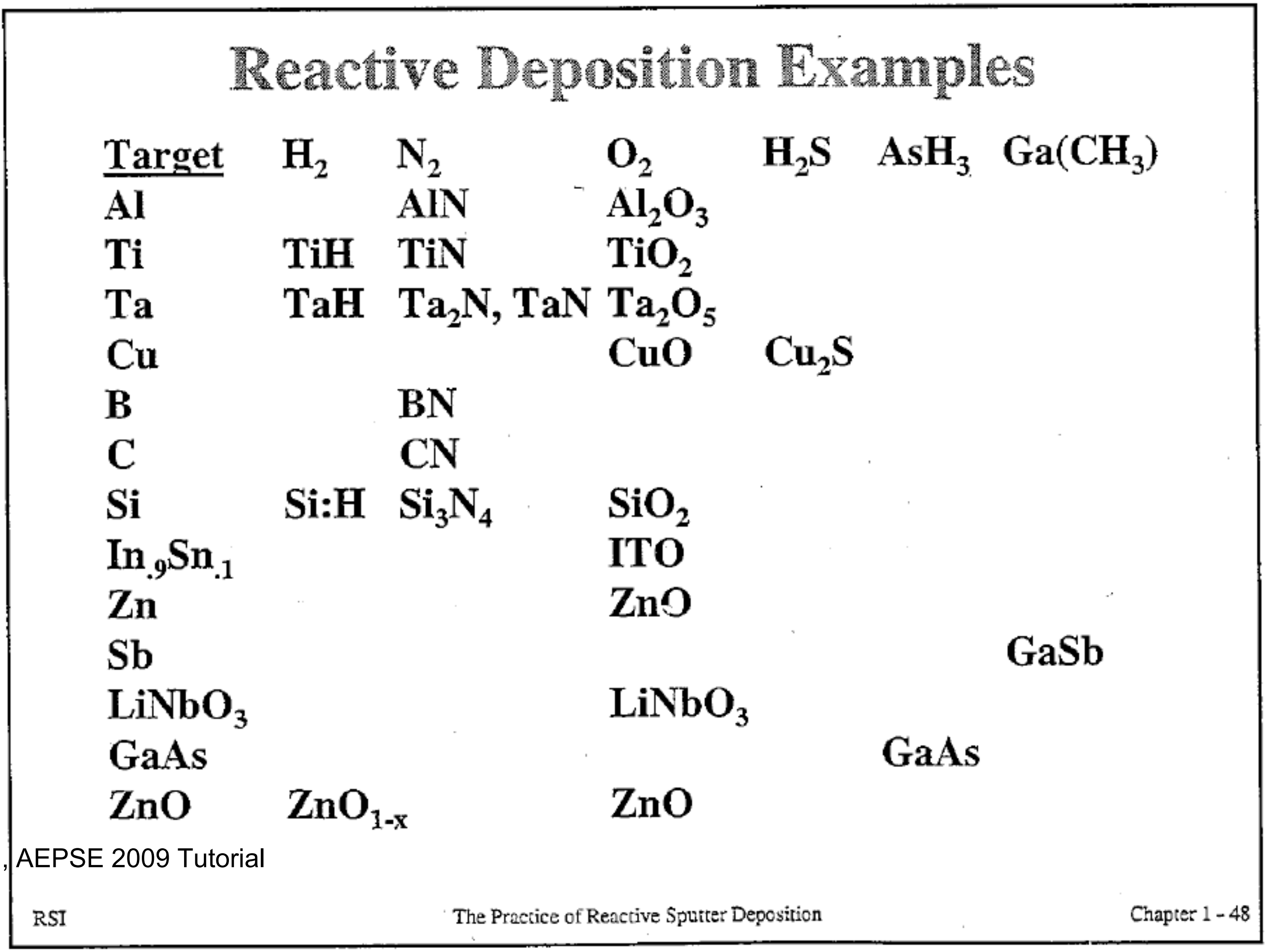
Reactive sputtering



Reactive Deposition Examples

Target	H_2	N_2	O_2	H_2S	AsH_3	$Ga(CH_3)$
Al		AlN	Al_2O_3			
Ti	TiH	TiN	TiO_2			
Ta	TaH	Ta_2N, TaN	Ta_2O_5			
Cu			CuO	Cu_2S		
B		BN				
C		CN				
Si	Si:H	Si_3N_4	SiO_2			
$In_{.9}Sn_{.1}$			ITO			
Zn			ZnO			
Sb						GaSb
$LiNbO_3$			$LiNbO_3$			
GaAs					GaAs	
ZnO	ZnO_{1-x}		ZnO			

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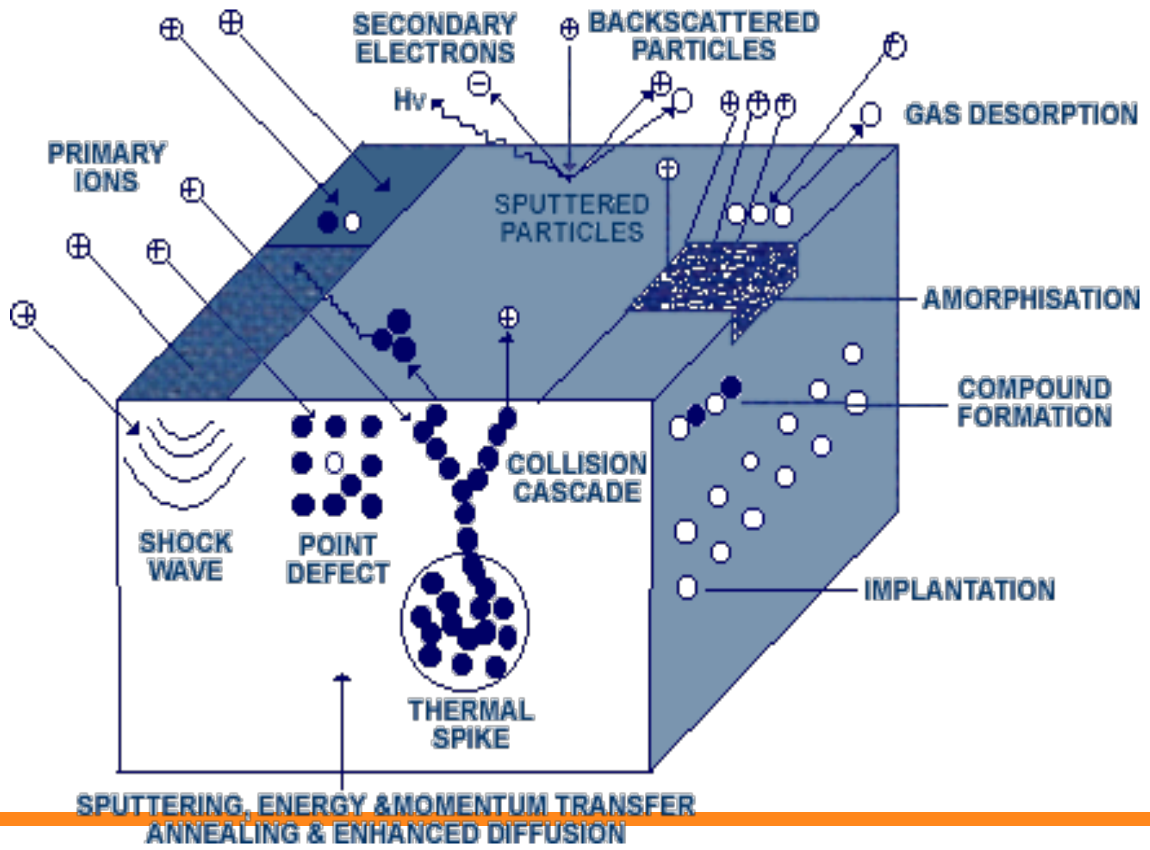
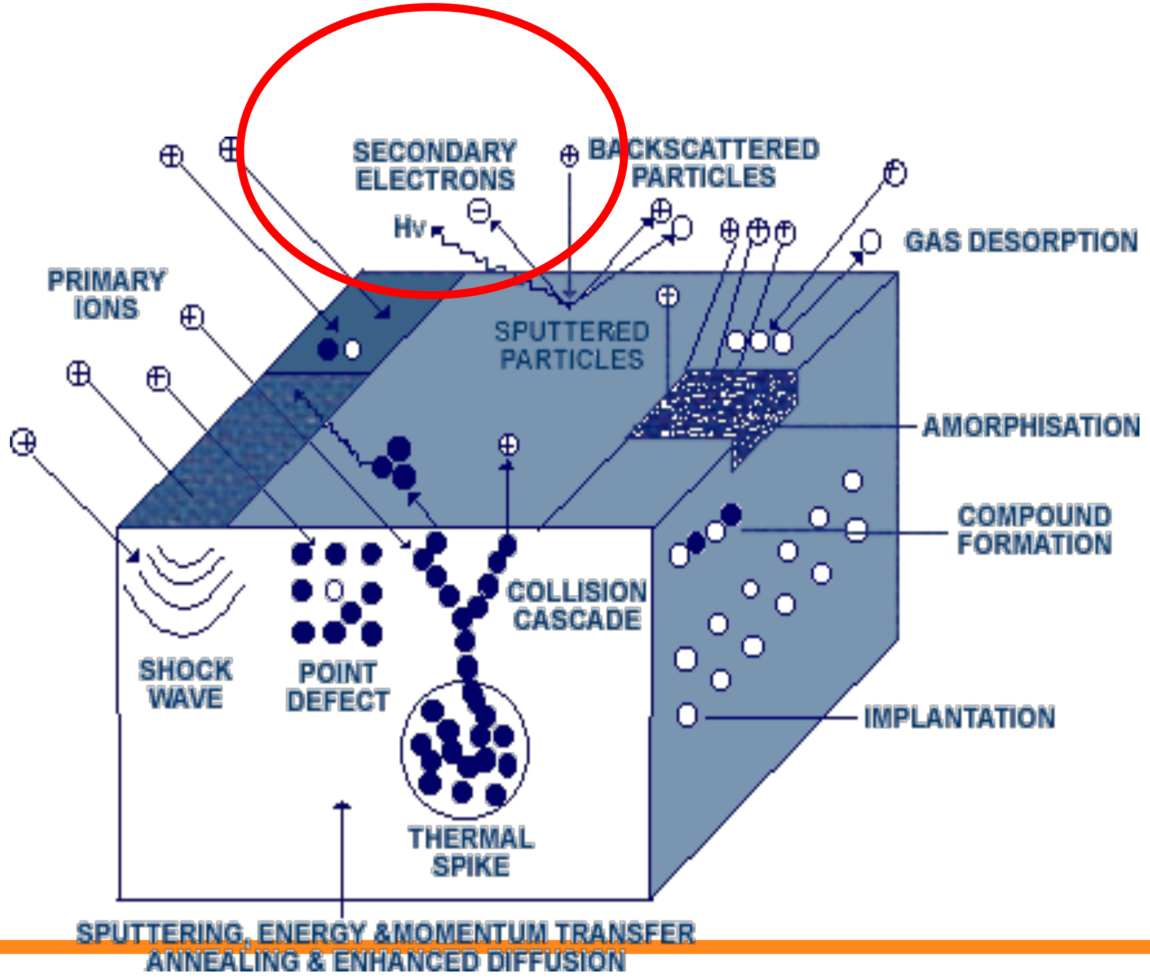
Ion solid interarctions

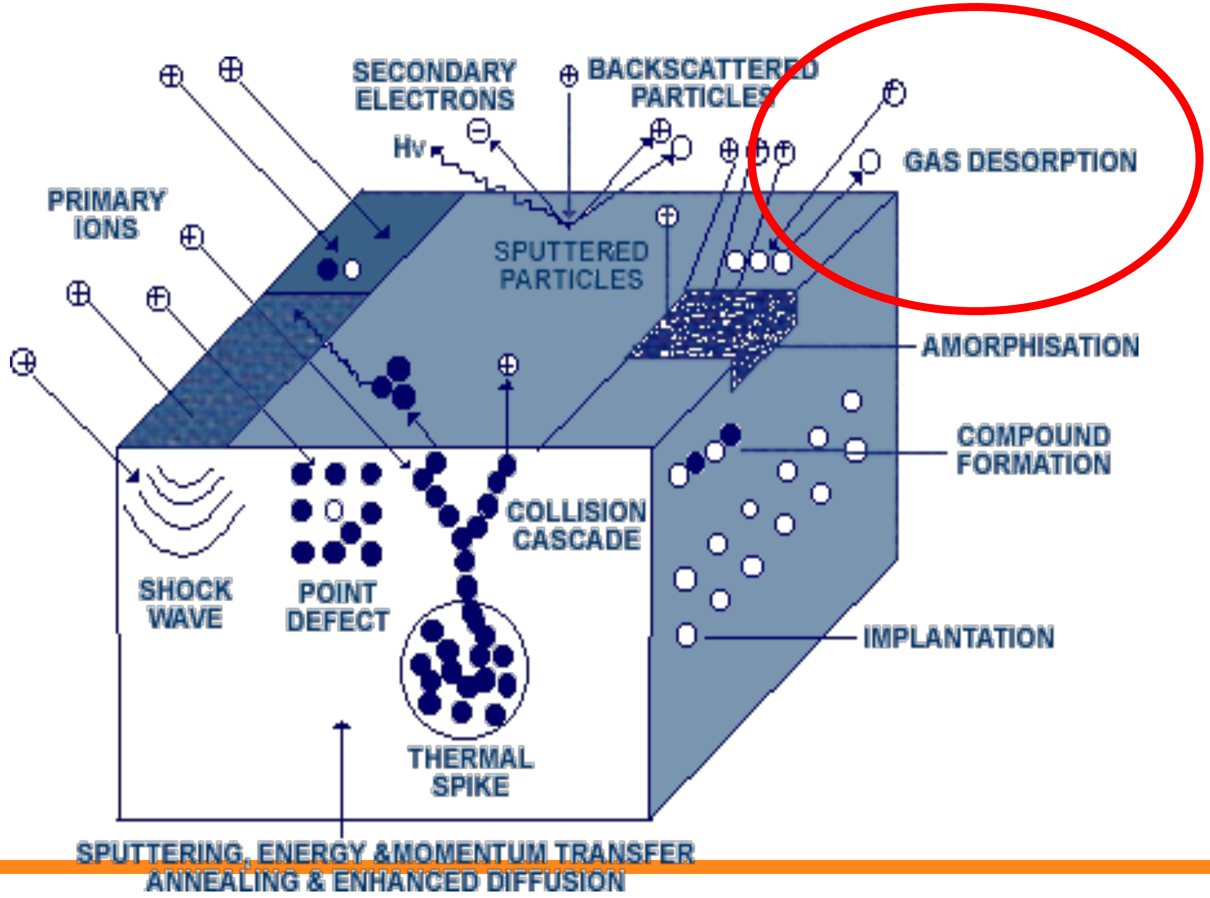
Energetic ion surface interactions



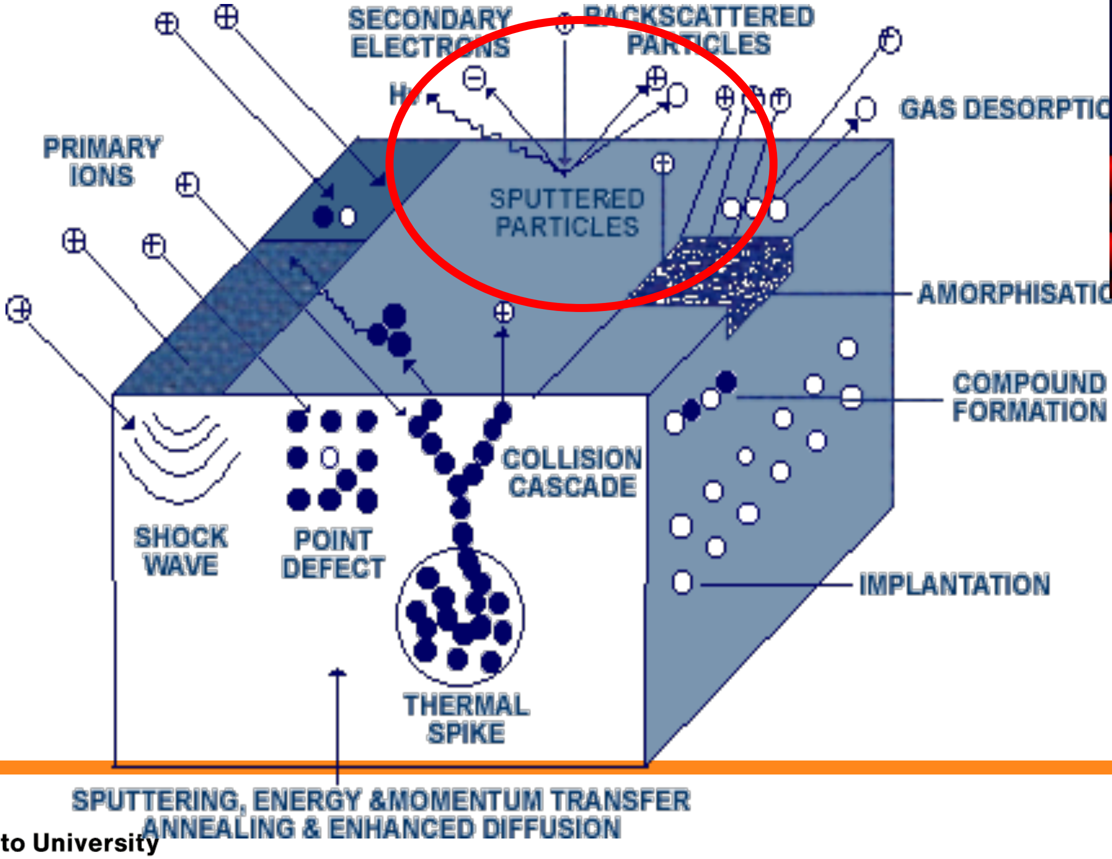
Secondary electrons

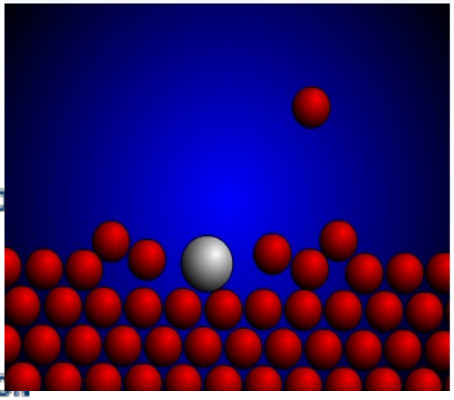


Desorption, cleaning

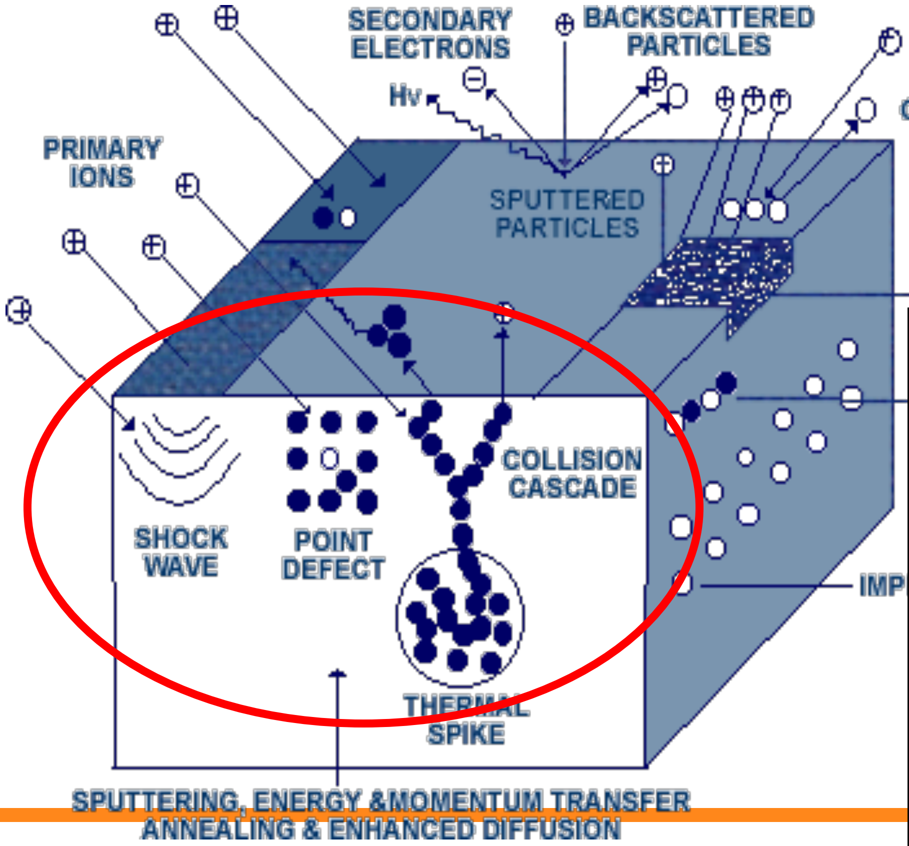


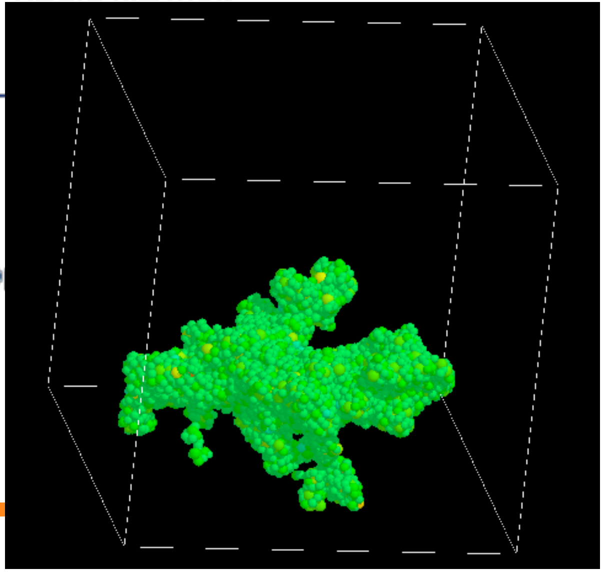
Sputtering


SECONDARY ELECTRONS
BACKSCATTERED PARTICLES
H
PRIMARY IONS
SPUTTERED PARTICLES
GAS DESORPTIO
AMORPHISATIO
COMPOUND FORMATION
COLLISION CASCADE
SHOCK WAVE
POINT DEFECT
THERMAL SPIKE
IMPLANTATION
SPUTTERING, ENERGY &MOMENTUM TRANSFER
ANNEALING & ENHANCED DIFFUSION



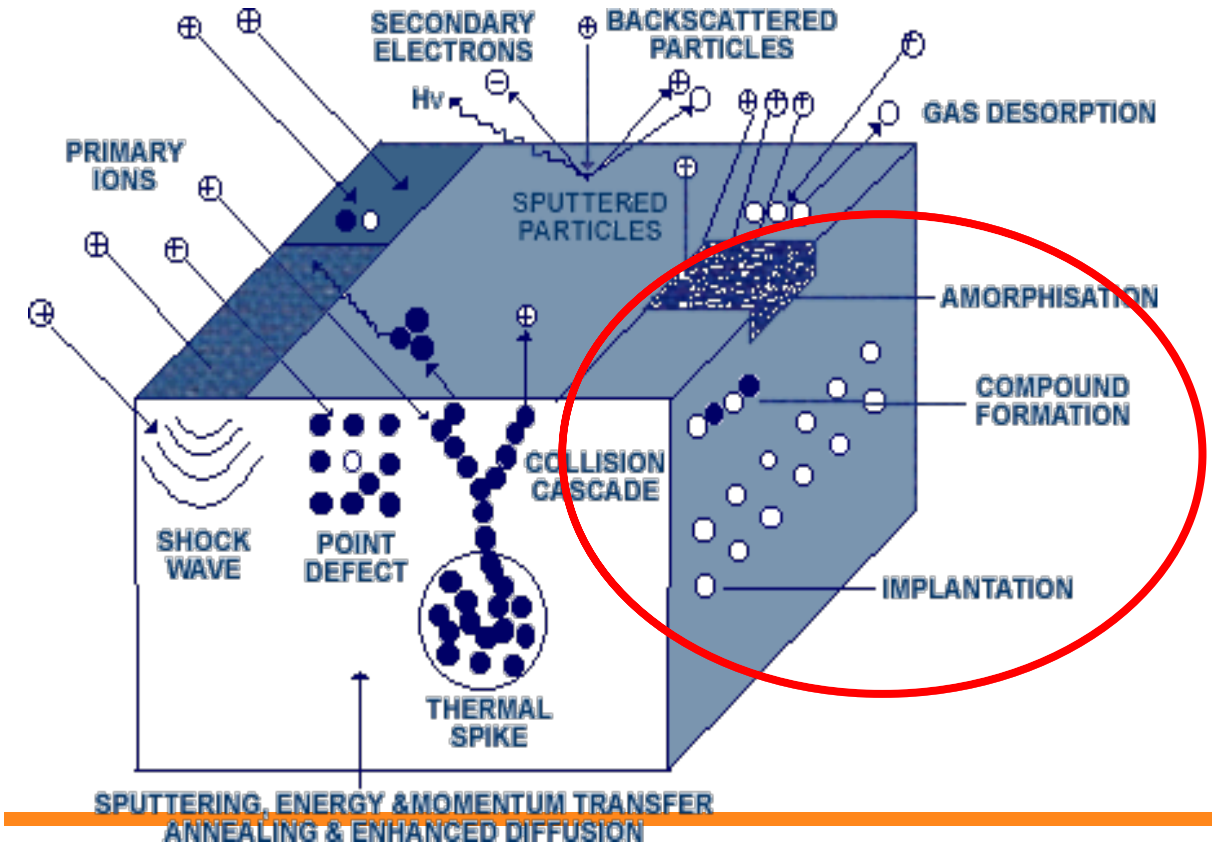
Collision cascade, thermal spike

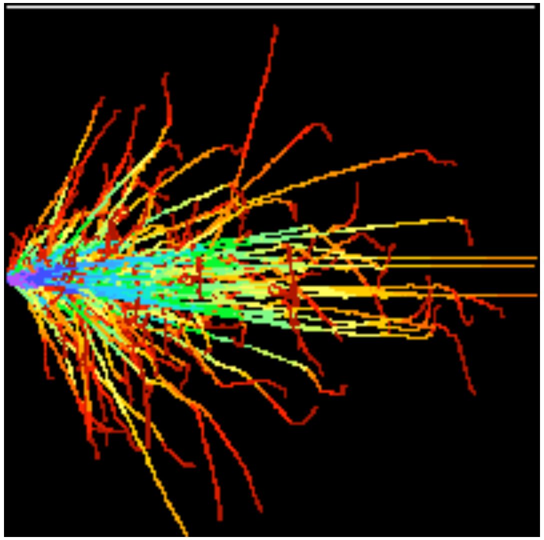




K. Nordlund

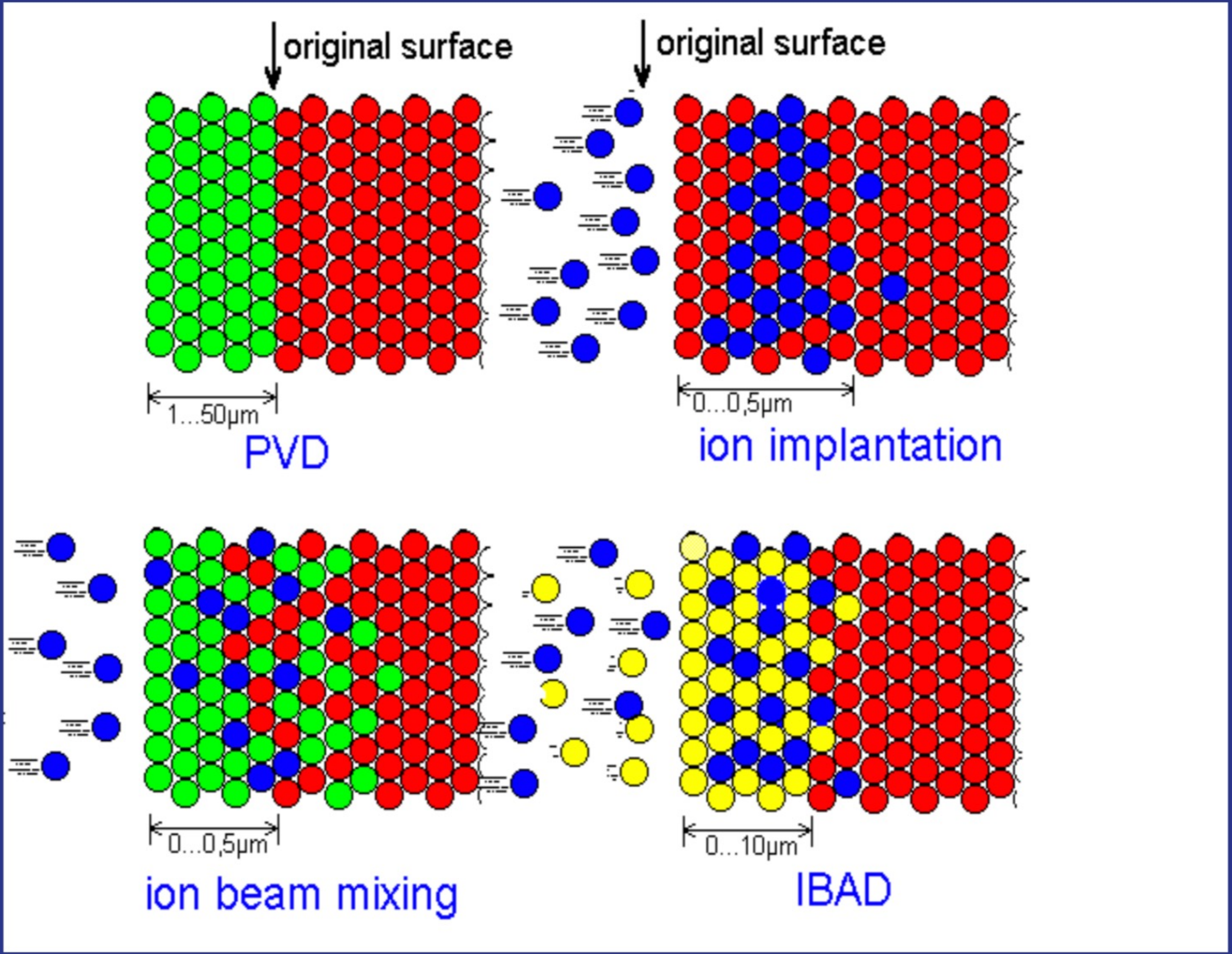
doping, compounds





PVD and Ion Assisted Processes

Which role can energetic ions play



Sputtering

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

Sigmund Theory

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

Good for low energy (<1keV)

where :

α is a function of M(target)/M(ion) and

incident angle $0.1 > \alpha > 1.4$

but often has a value of 0.2 - 0.4

M1 is the Mass of the ion

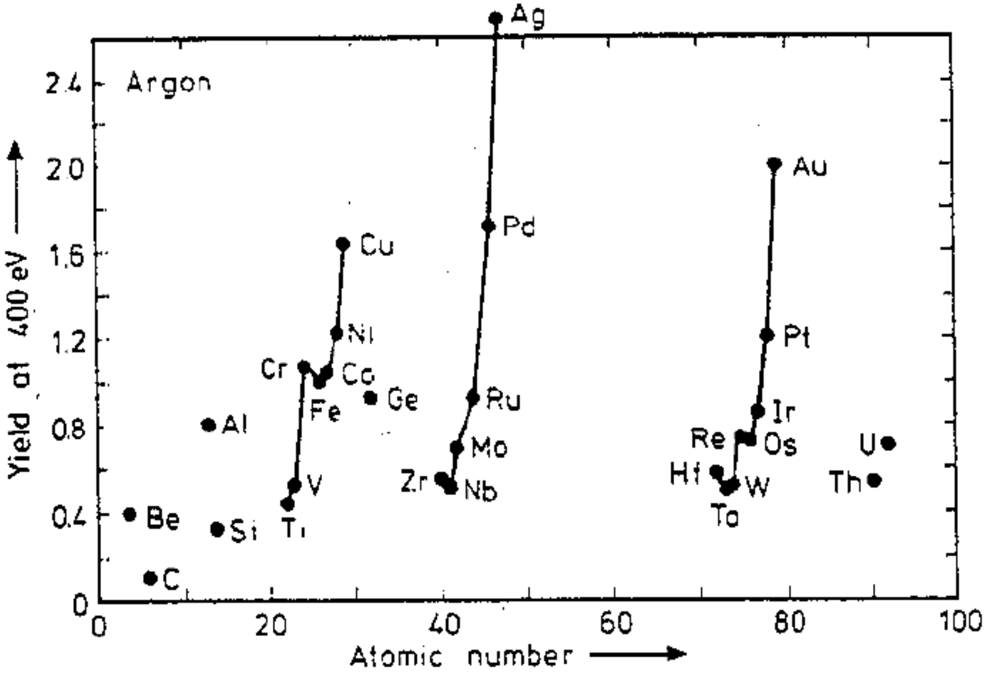
M2 is the mass of the target

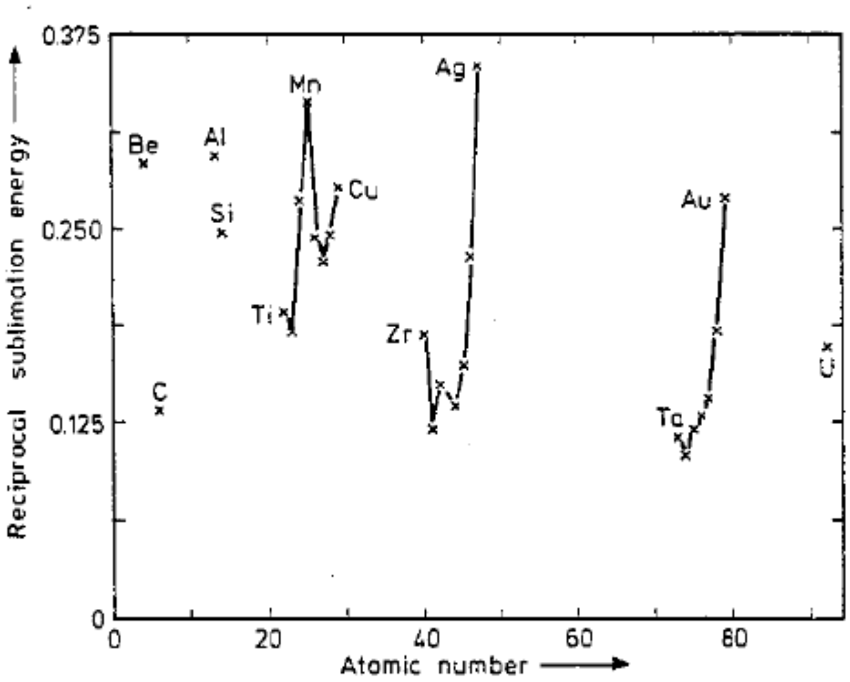
E is incident ion energy

Us is the binding energy of the target ions

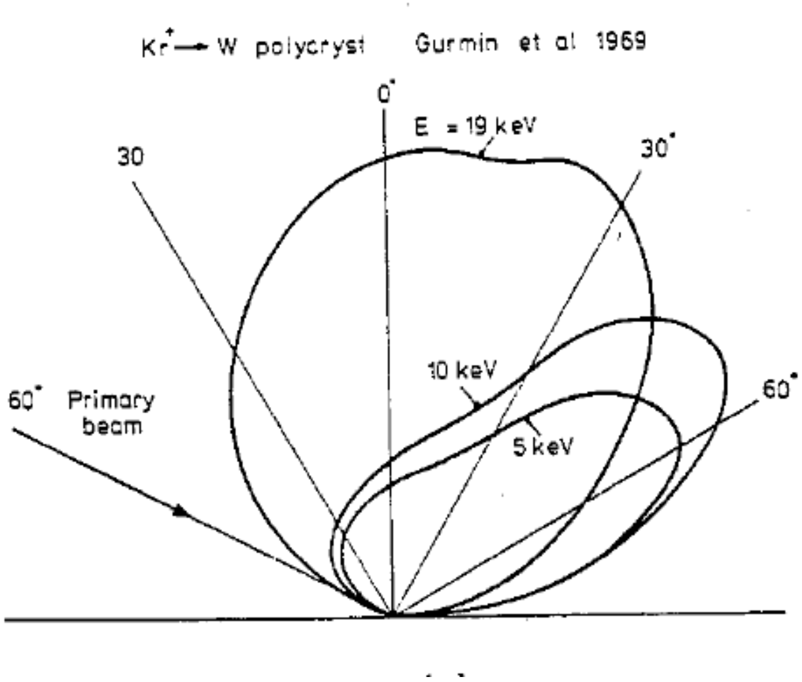
Sputter yield and sublimation energy

$$N(E) \propto \frac{E}{(E+U_0)}$$





Sputter yield angle dependence



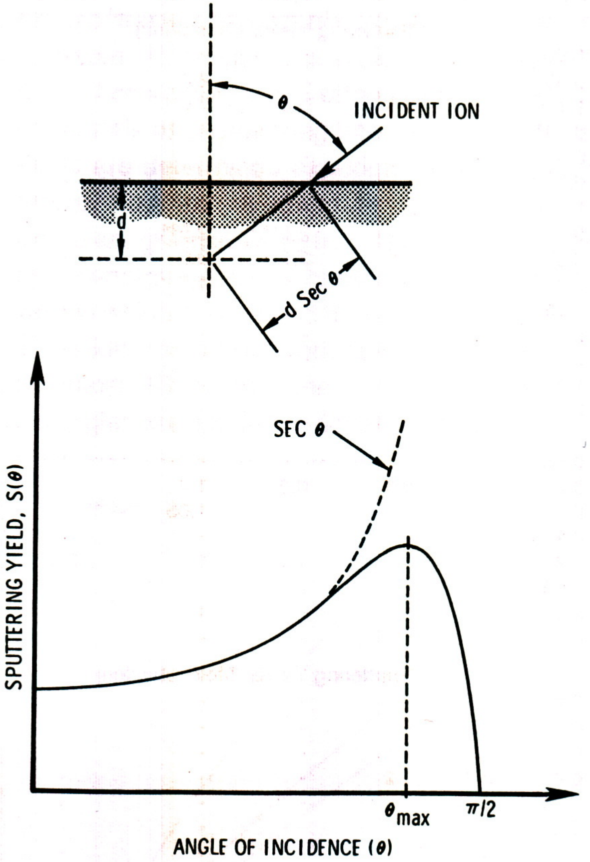


Figure 5.7. Schematic diagram showing variation of the sputtering yield with ion angle of incidence for a constant ion energy.

Sputter yi ibution

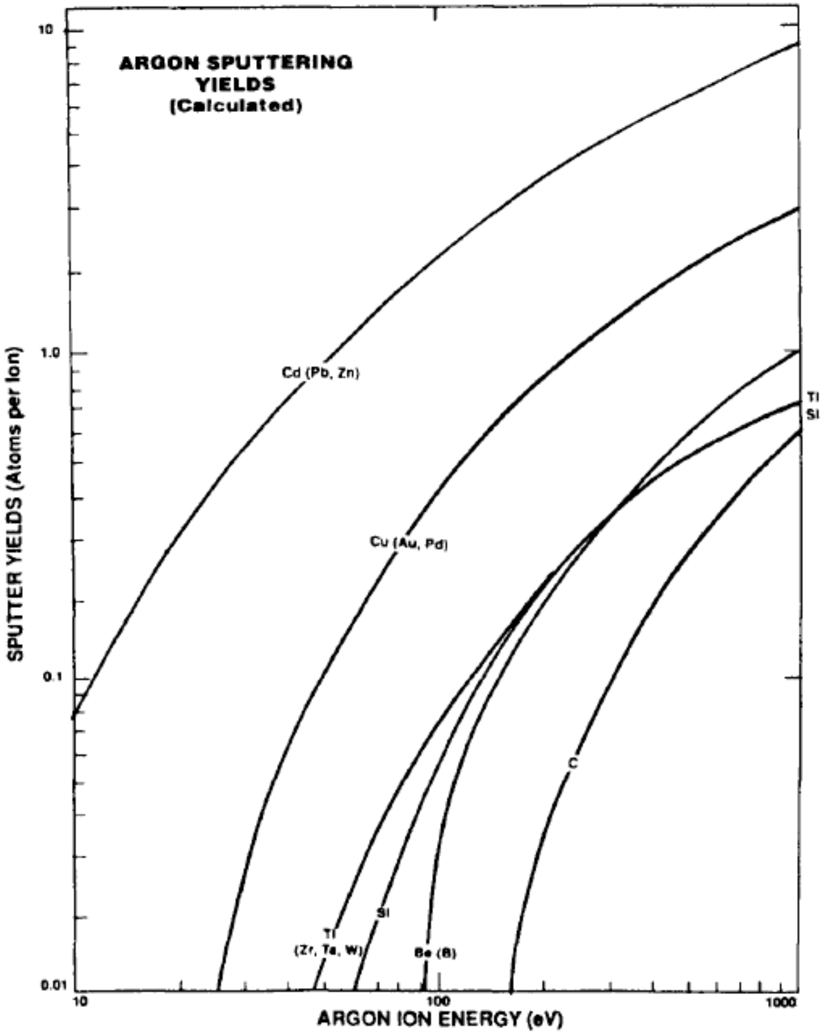
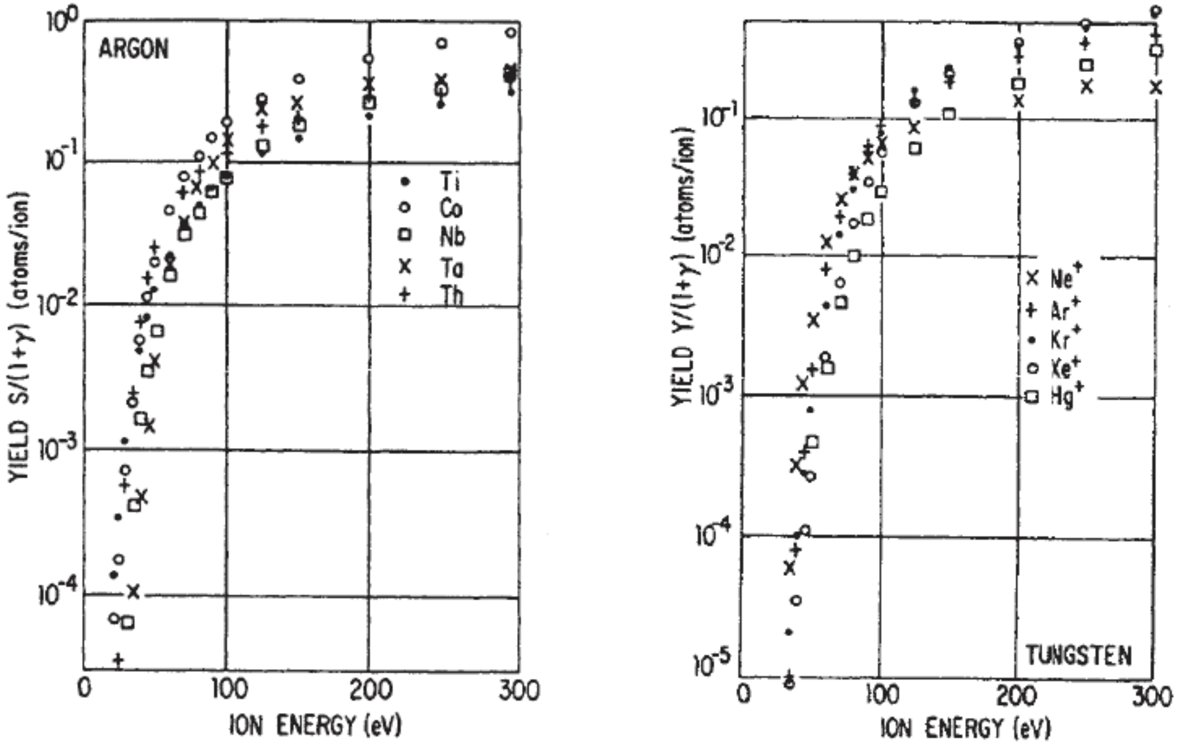


Figure 6-3. Some calculated sputtering yields (adapted from Ref. 20).

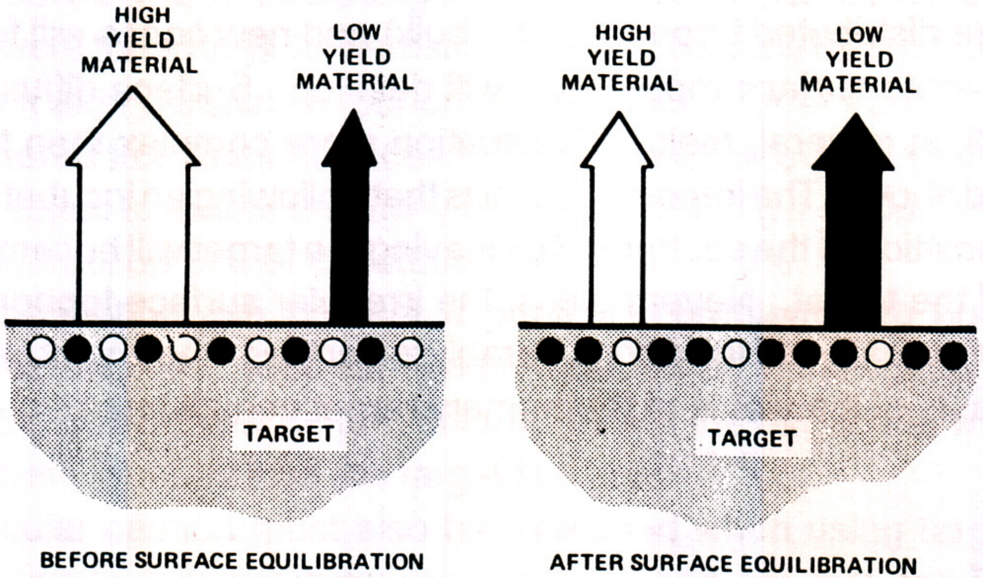
Sputter yield angle dependence and energy distribution



(a) (b)

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

Preferential sputtering



BEFORE SURFACE EQUILIBRATION

AFTER SURFACE EQUILIBRATION

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

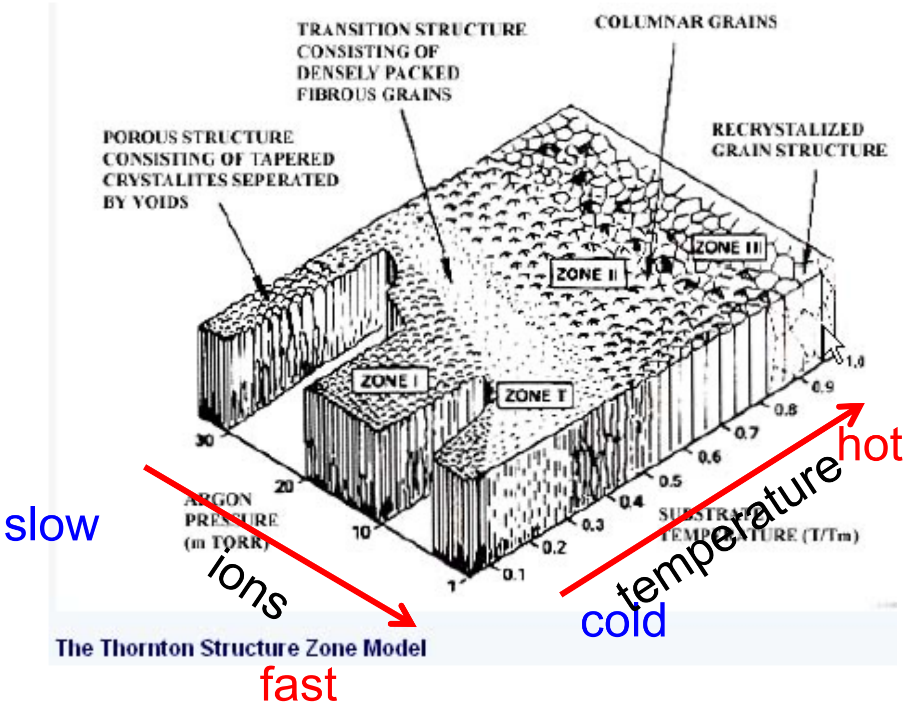
Adatom nucleation and surface diffusion processes

- 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



The Thornton Structure Zone Model

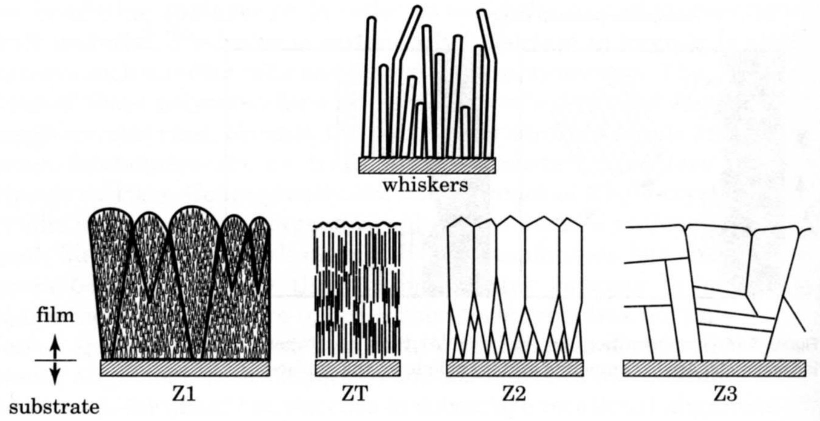


Figure 5.15 Characteristics of the four basic structural zones and of whiskers, in cross section. The ratio of substrate T to film melting T (T_s/T_m) increases in the direction Z1→ZT→Z2→Z3.

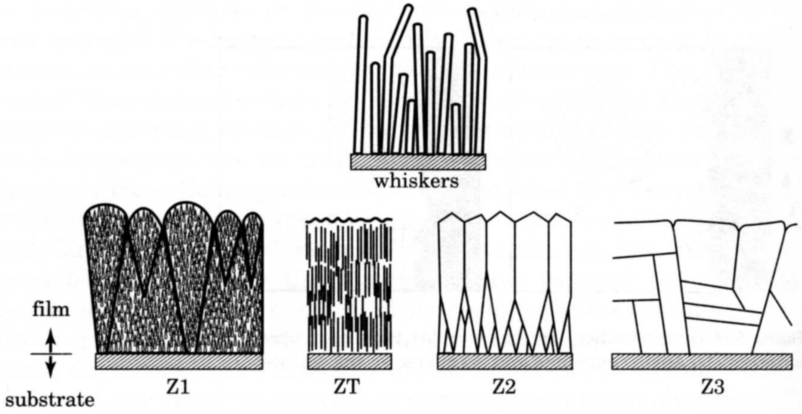


Figure 5.15 Characteristics of the four basic structural zones and of whiskers, in cross section. The ratio of substrate T to film melting T (T_s/T_m) increases in the direction Z1→ZT→Z2→Z3.

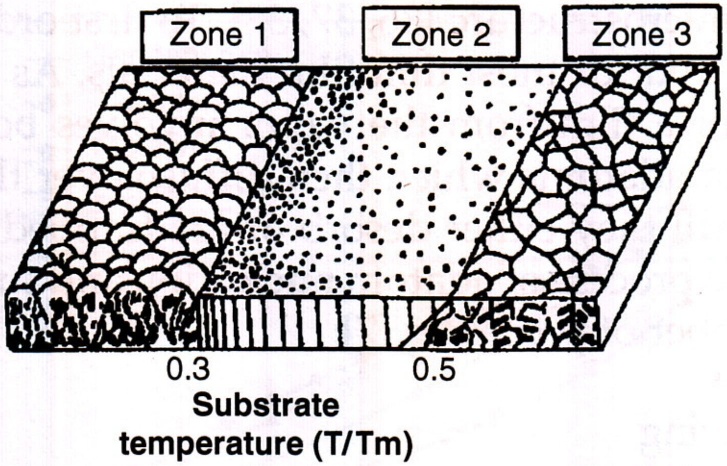


Figure 3.26 Structure zone model of Movechan and Demchishin [39].

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

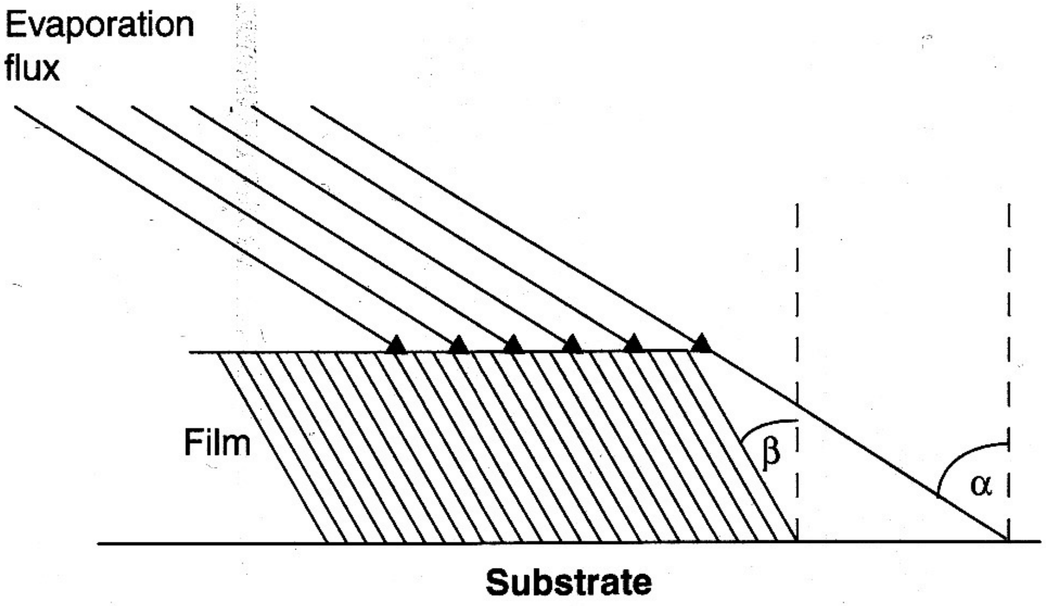


Figure 3.20 Geometry used in the tangent rule [29].


6.2.2012 Koskinen

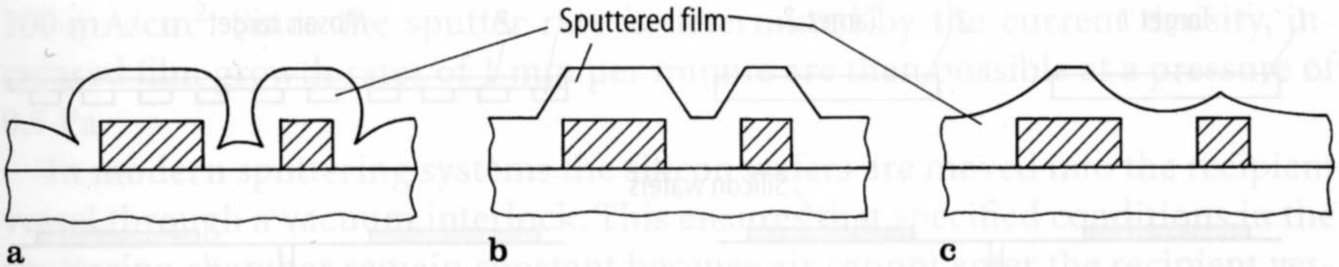


Fig. 3.1.19a-c. Edge coverage of sputtered layers: **a** no bias; **b** moderate bias; **c** heavily biased

Structural hierarchy

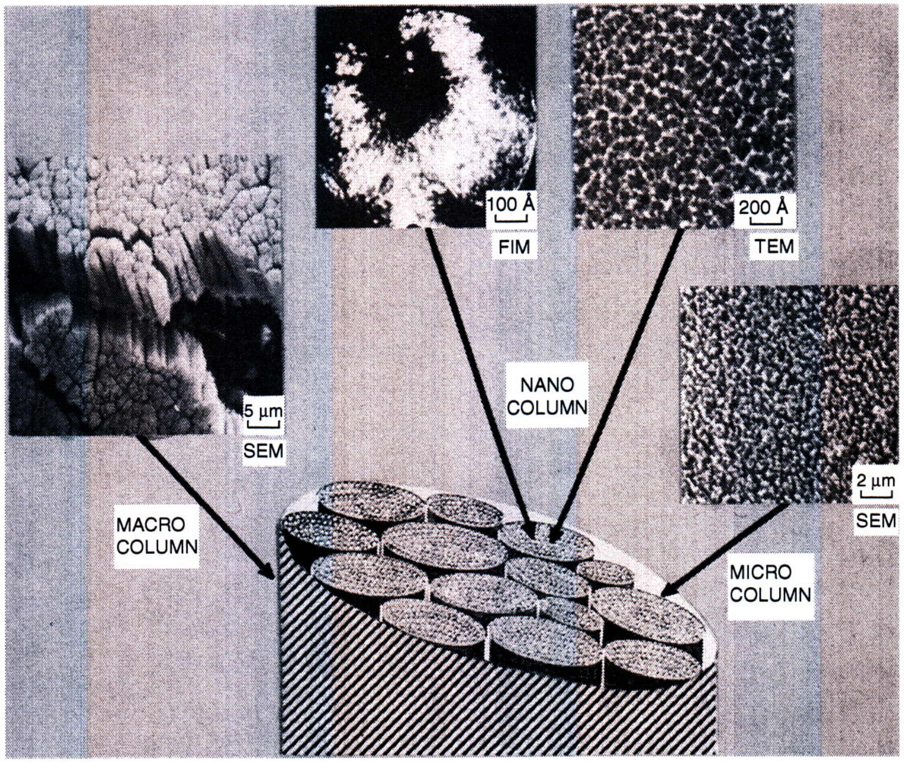


Figure 3.22 Physical structure of nano-, micro and macro columns in a-Ge films [31].

Nodules

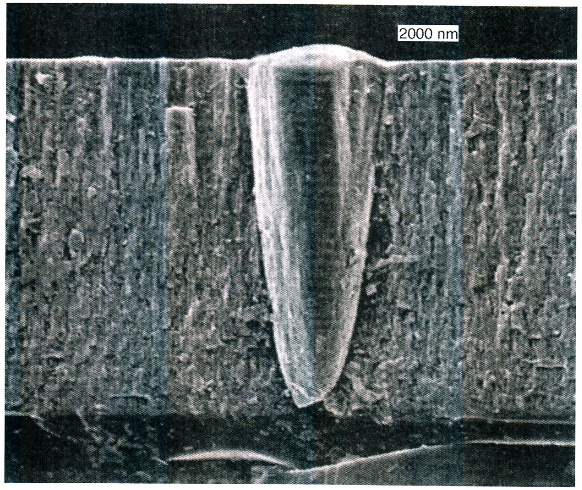


Figure 3.23 Nodule in and AlON rugate filter [28].

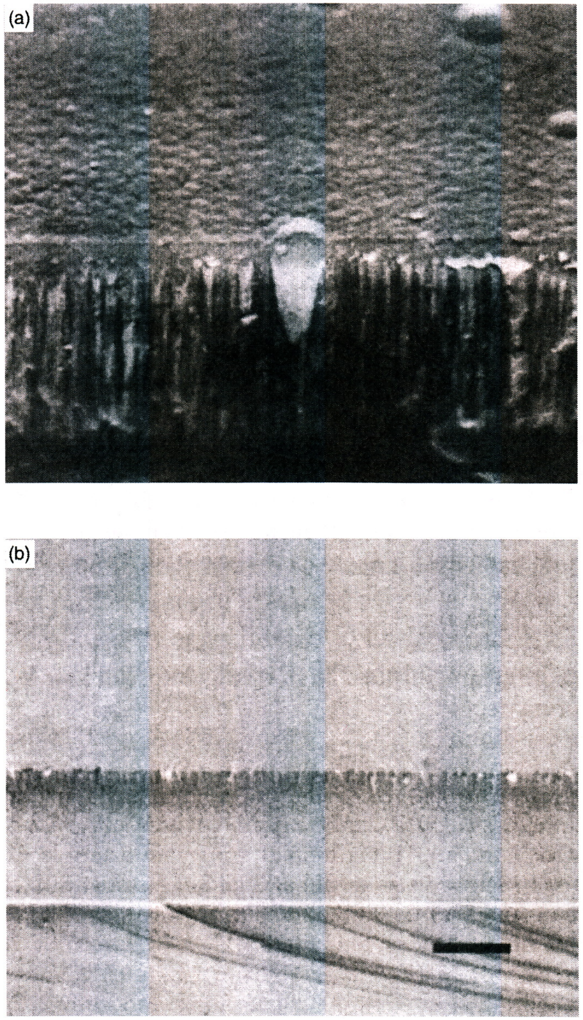


Figure 3.21 SEM micrograph of two SiC films; film (a) had no ion bombardment and film (b) was exposed to ion bombardment [31].

GLAD

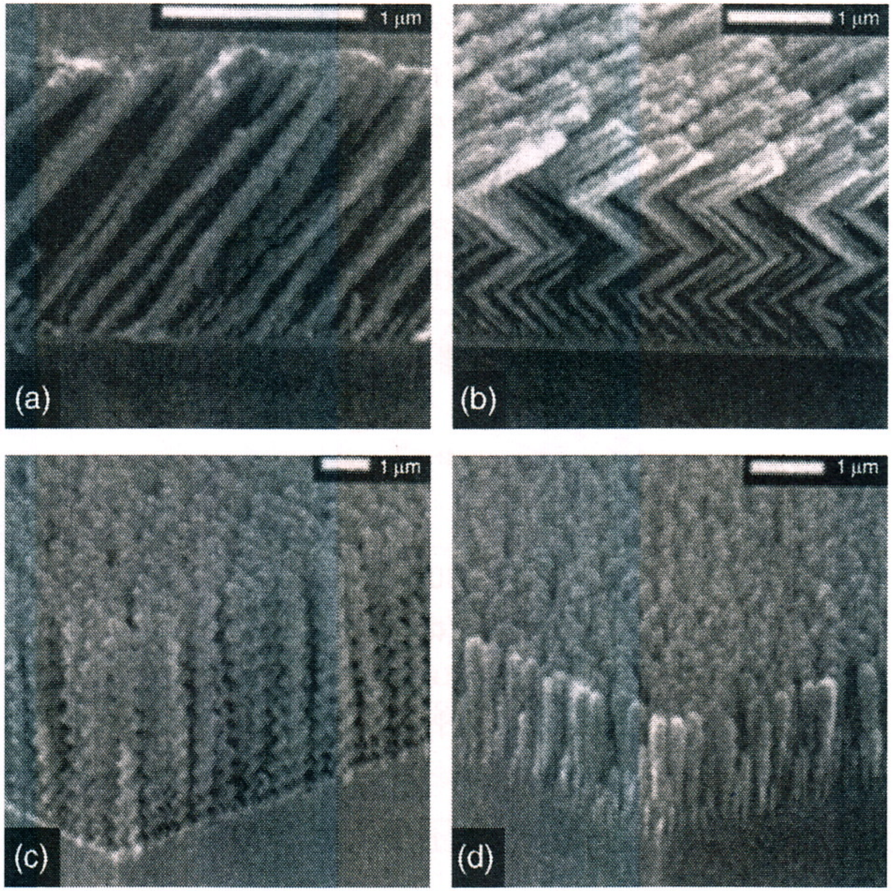


Figure 3.24 Columnar structures fabricated using the GLAD process [32].

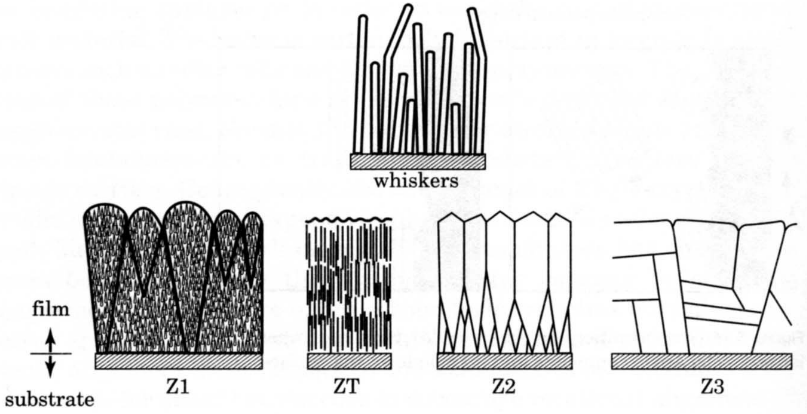


Figure 5.15 Characteristics of the four basic structural zones and of whiskers, in cross section. The ratio of substrate T to film melting T (T_s/T_m) increases in the direction Z1→ZT→Z2→Z3.

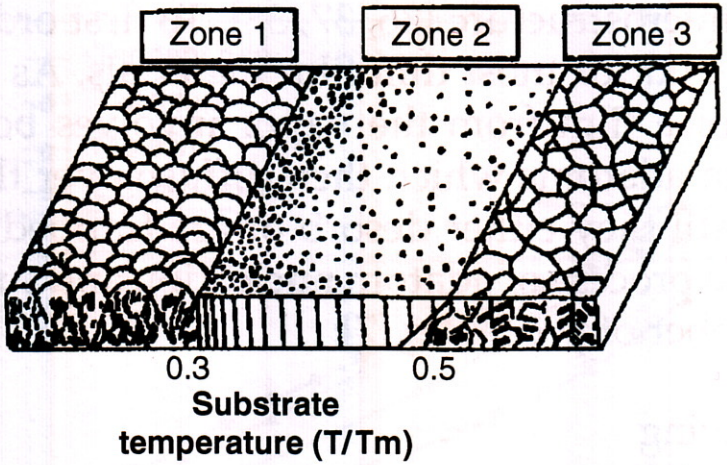


Figure 3.26 Structure zone model of Movechan and Demchishin [39].

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 2surface 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

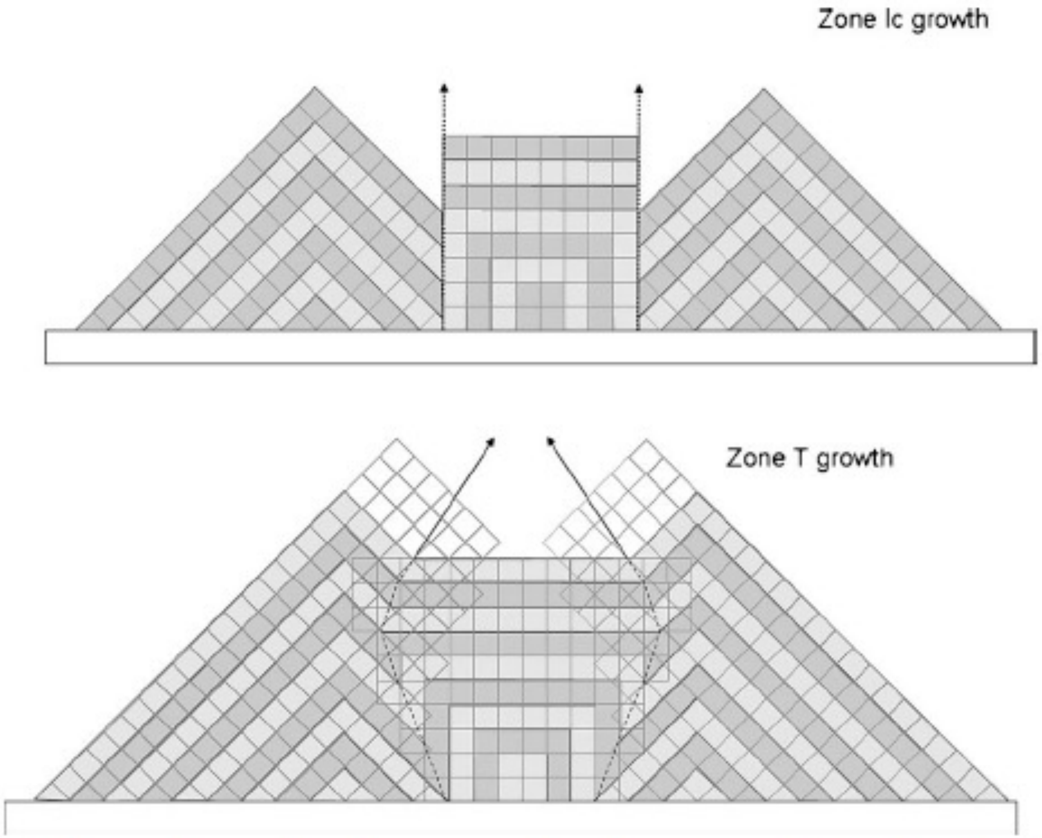


Figure 5.21: Schematic comparison between zone Ic and zone T growth. To indicate the identical normal growth rate of the planes of both grains, alternating coloring is used. In zone T, an overgrowth of one grain by an adjacent grain is observed.

Columnar growth

AlN piezoelectric film

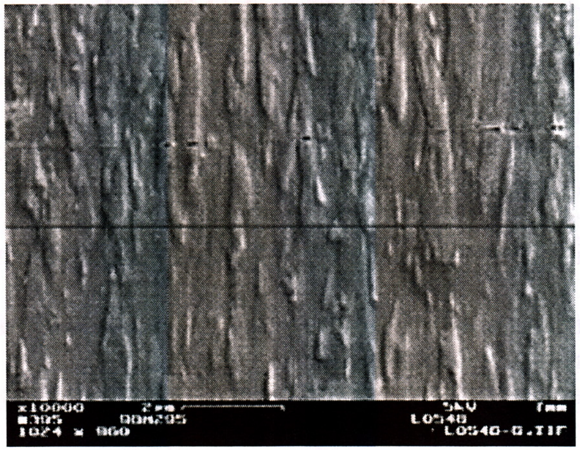


Figure 3.18 SEM picture of well-behaved columnar thin film microstructure.

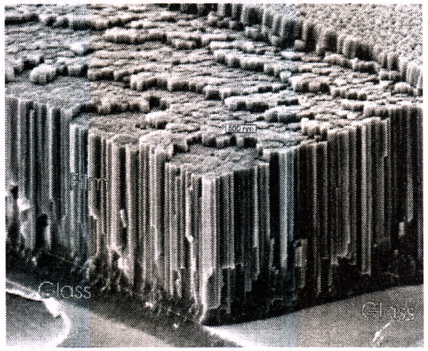


Figure 3.19 Columnar structure in an RF sputtered ALON film [28].

Columnar crystals

15.4.2011 Koskinen

Columnar crystals


15.4.2011 Koskinen

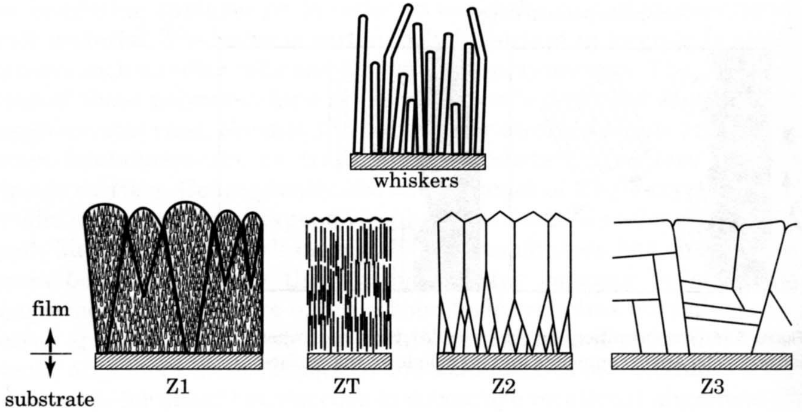


Figure 5.15 Characteristics of the four basic structural zones and of whiskers, in cross section. The ratio of substrate T to film melting T (T_s/T_m) increases in the direction Z1→ZT→Z2→Z3.

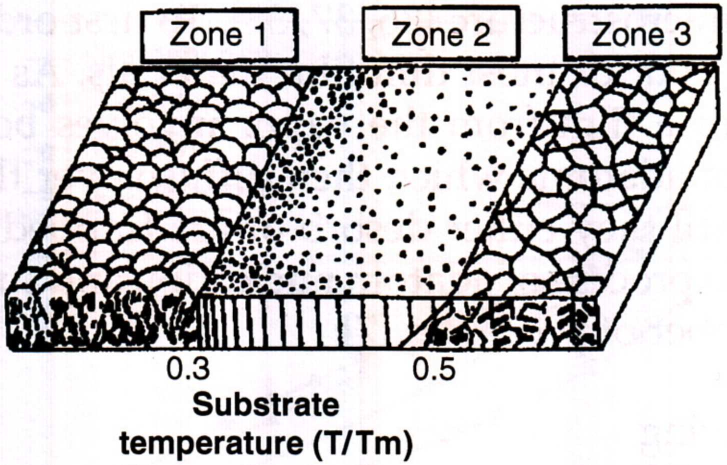


Figure 3.26 Structure zone model of Movechan and Demchishin [39].

Zone 3
- bulk diffusion dominates
- recrystallization of large crystals

Effect of ion energy

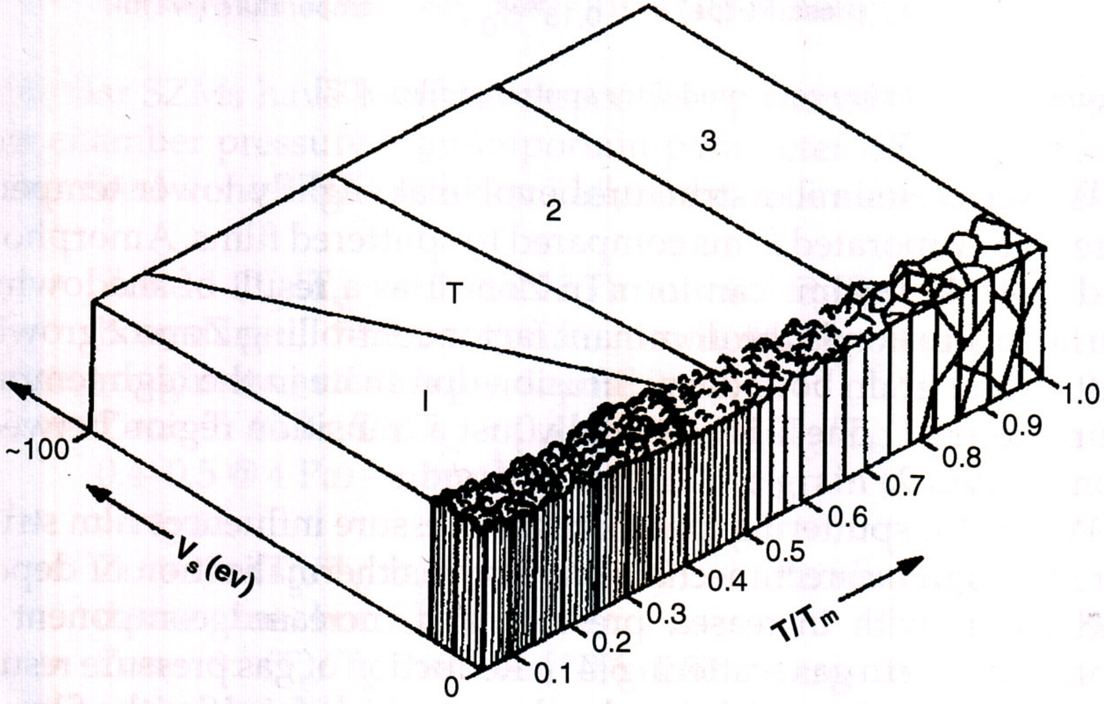


Figure 3.28 Revised SZD for RF sputtering, including ion bombardment.

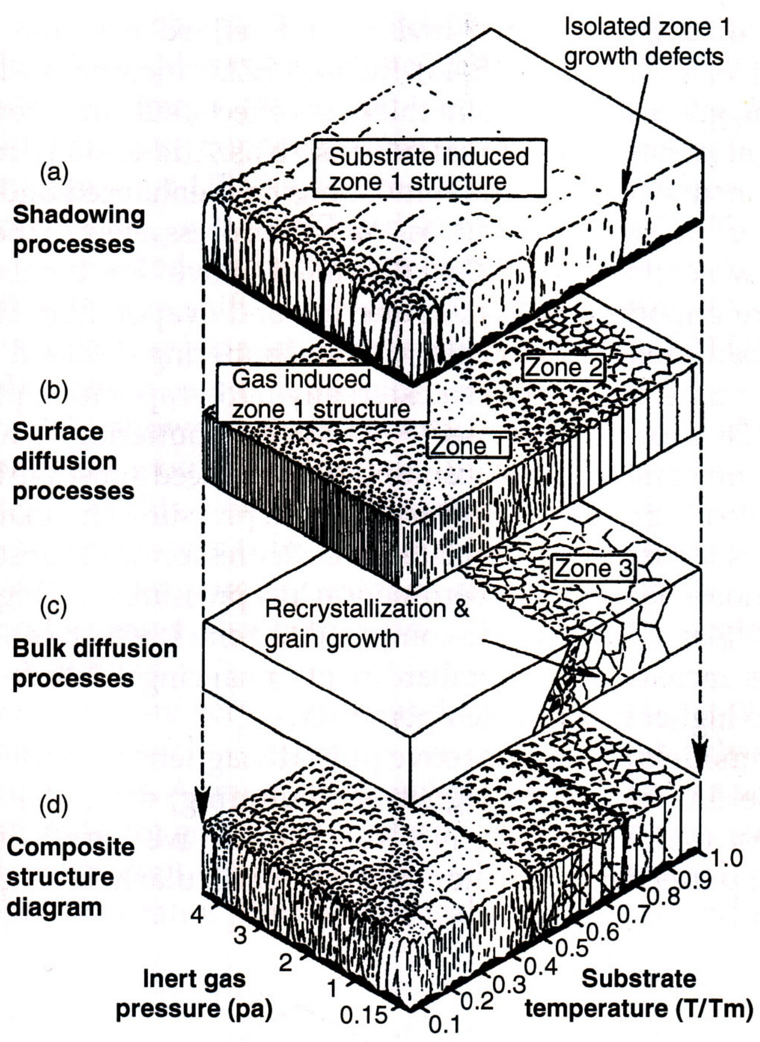
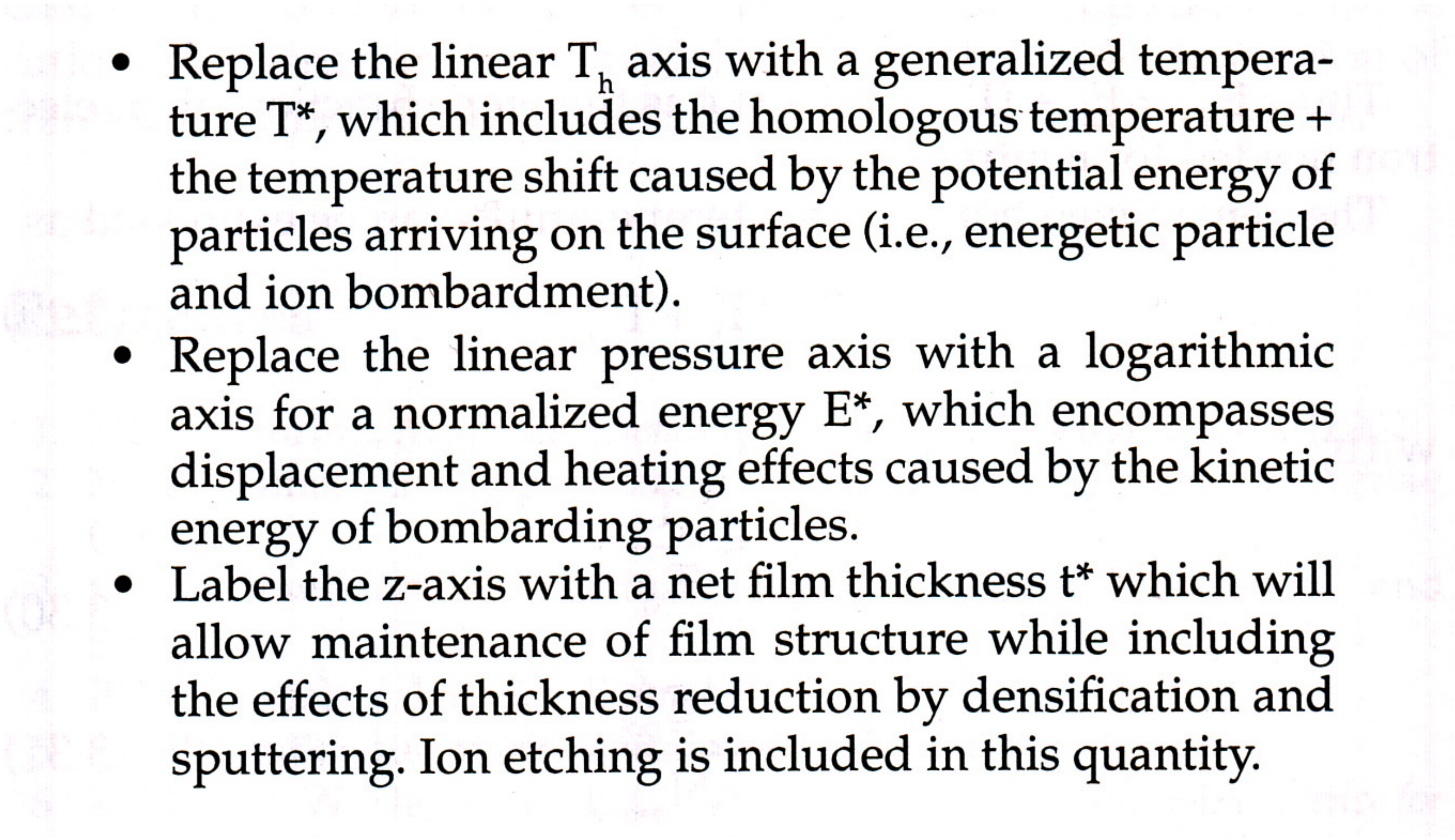


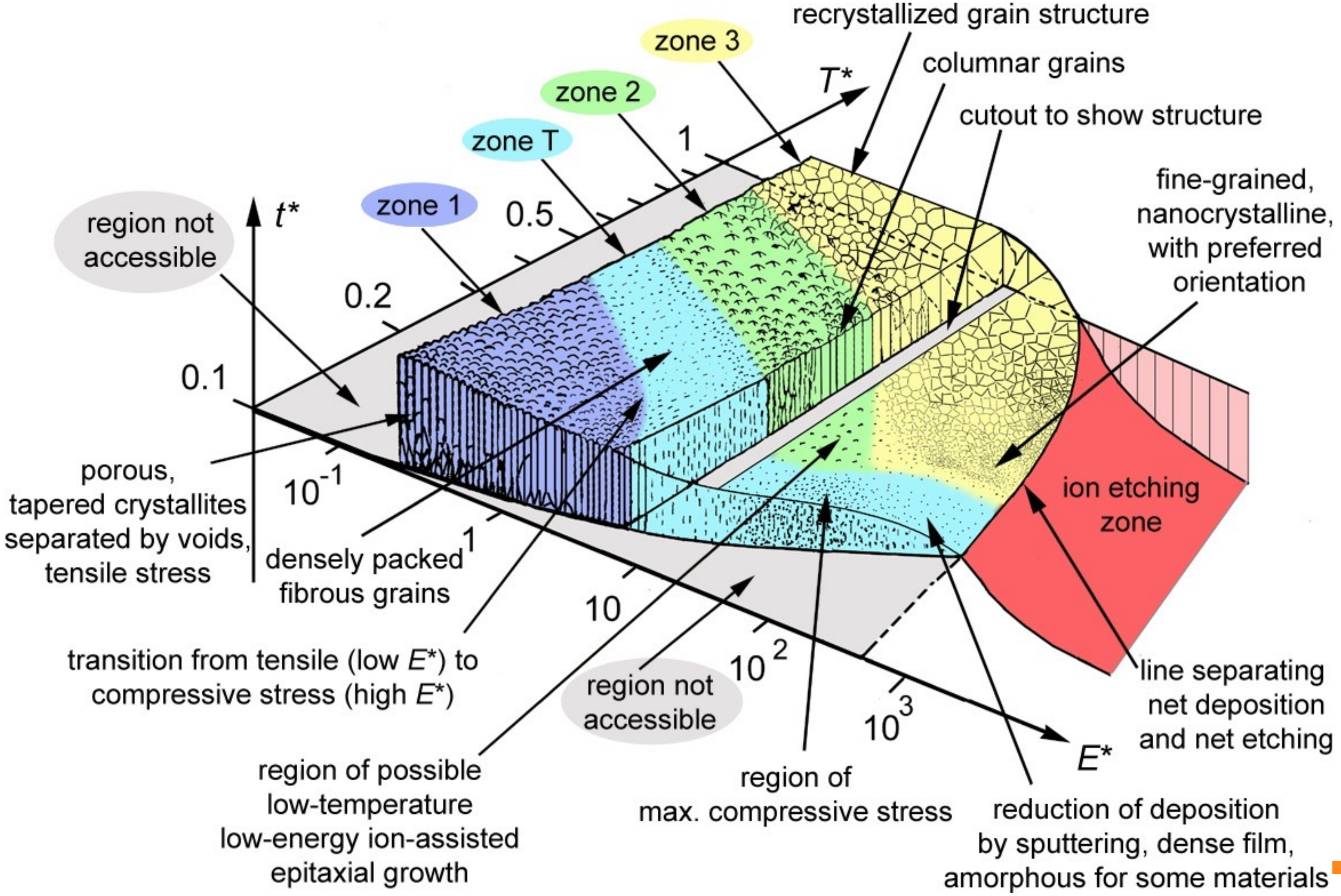
Figure 3.27 Structure zone model for sputtered films [37].

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 Thorton diagram



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Reduced parameters SZD

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

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

- 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_{kin} ion kinetic energy
- E_o plasma potential
- V_{sheath} sheath potential
- ø electron work function (c. 4 eV)
- J_a, flux of species a
- m_a, mass of incoming atom
- m_s, mass of surbstrate
- k, Bolzmann constant
- N_{moved}, number of rearranged atoms

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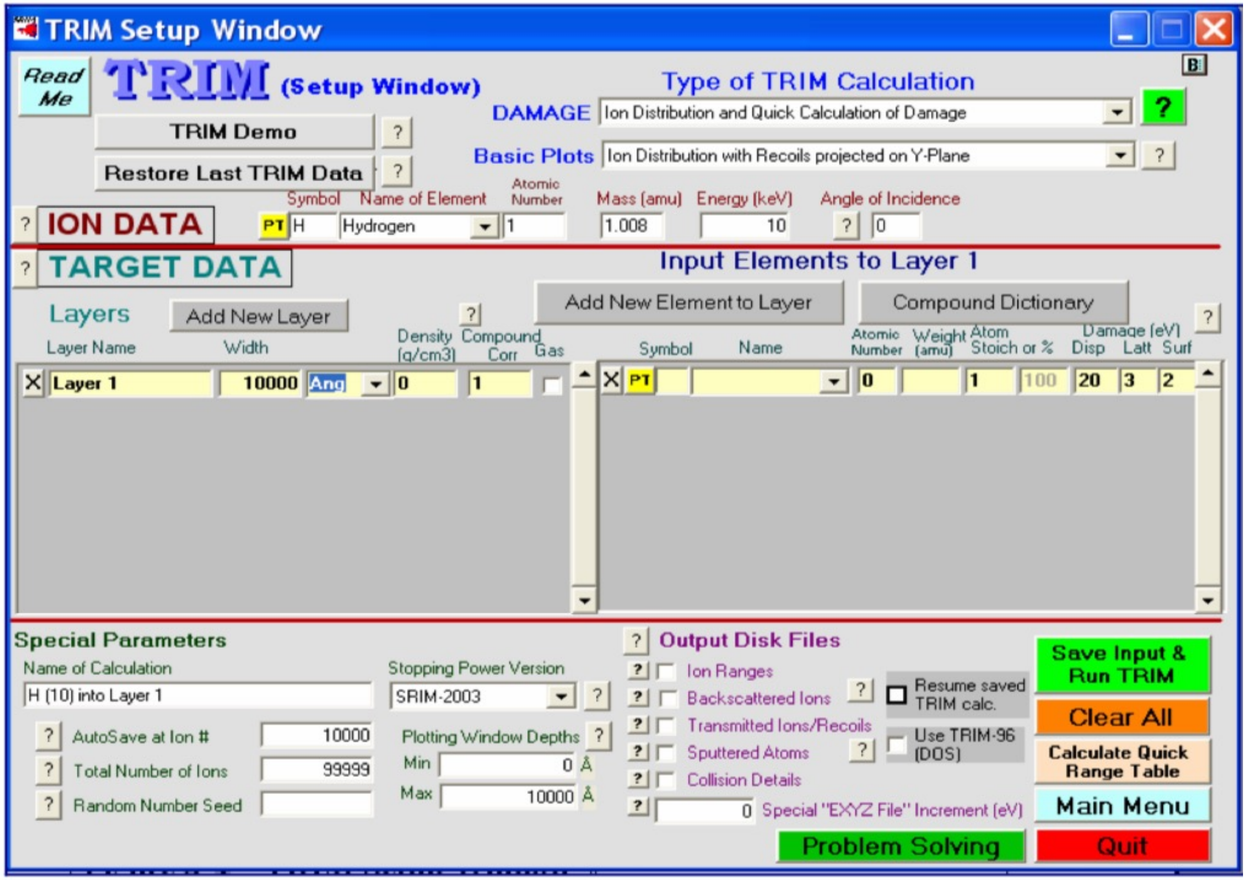
TRIM and SRIM simulations

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



Type of TRIM Calculation

DAMAGE: Ion Distribution and Quick Calculation of Damage

Basic Plots: Ion Distribution with Recoils projected on Y-Plane

ION DATA

Symbol	Name of Element	Atomic Number	Mass (amu)	Energy (keV)	Angle of Incidence
H	Hydrogen	1	1.008	10	0

TARGET DATA

Layers

Layer Name	Width		Density (g/cm3)	Compound Corr	Gas
Layer 1	10000	Ang	0	1	☐

Input Elements to Layer 1

Symbol	Name	Atomic Number	Weight (amu)	Atom Stoich	or %	Damage (eV) Disp	Latt	Surf
PT		0		1	100	20	3	2

Special Parameters

Name of Calculation: H (10) into Layer 1

Stopping Power Version: SRIM-2003

AutoSave at Ion #: 10000

Total Number of Ions: 99999

Random Number Seed:

Plotting Window Depths: Min 0 Å, Max 10000 Å

Output Disk Files

- ☐ Ion Ranges
- ☐ Backscattered Ions
- ☐ Transmitted Ions/Recoils
- ☐ Sputtered Atoms
- ☐ Collision Details
- 0 Special "EXYZ File" Increment (eV)

☐ Resume saved TRIM calc.

☐ Use TRIM-96 (DOS)