EPFL

MICRO-435 Quantum and Nanocomputing

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HT FABRICATION : PART 2

MOLECULAR TRANSISTOR FABRICATION

OBJECTIVES

a) EM PHYSICAL MODELING

b) FAVOURING "GOOD" EM

c) N.G. ARRAY BASED ON EM

2) EM PHYSICAL MODELING

EM EXPLANATION

STARTING POINT: { THERMODINAMICS OF IRREVERSIBLE ROCESSES

3 FLUXES

J_e ELECTRON FLUX

J_m METAL ION FLUX

J_u ENERGY FLUX

} INDUCED BY {

3 FORCES OR POTENTIAL GRADIENTS

X_k

$k: e, m, u$

LET'S STOP A MOMENT TO SEE THE FORCES AND PARAMETERS INVOLVED for k

e, m

$$X_k = -\nabla \mu^k_{ec}$$

POTENTIAL GRADIEN

ELECTROCHEMICAL POTENTIAL

$$\mu^k_{ec} = \mu + z \cdot e \cdot \varphi$$

φ → electrostatic potential

μ → chemical potential

z → particle charge → −1 el. ; → +1 IONS

for X_u local temperature gradient

GENERAL DESCRIPTION OF THE SYSTEM

$$
\begin{cases}
J_m = -L_{m,m} \nabla\left(\frac{\mu^m_{ec}}{T}\right) - L_{m,e} \nabla\left(\frac{\mu^e_{ec}}{T}\right) - L_{m,u}\left(\frac{\nabla T}{T^2}\right) \\
J_e = -L_{e,m} \nabla\left(\frac{\mu^m_{ec}}{T}\right) - L_{ee} \nabla\left(\frac{\mu^e_{ec}}{T}\right) - L_{e,u}\left(\frac{\nabla T}{T^2}\right) \\
J_u = -L_{u,m} \nabla\left(\frac{\mu^m_{ec}}{T}\right) - L_{u,e} \nabla\left(\frac{\mu^e_{ec}}{T}\right) - L_{e,u}\left(\frac{\nabla T}{T^2}\right)
\end{cases}
$$

$L_{i,j}$ phenomenological constant.

RELATE EACH FLUX TO ALL FORCES

DESCRIBES:
- ELECTROMIGRATION
- THERMO-ELECTRIC EFFECT
- THERMODIFFUSION

DEPENDING ON THE CASE SUBPARTS ARE MORE INVOLVED, OTHER NEGLECTED

GENERAL DESCRIPTION OF THE SYSTEM

$$
\begin{cases}
J_m = -L_{m,m} \nabla\left(\dfrac{\mu_{ec}^{m}}{T}\right) - L_{m,e} \nabla\left(\dfrac{\mu_{ec}^{e}}{T}\right) - L_{m,u}\left(\dfrac{\nabla T}{T^2}\right) \\
J_e = -L_{e,m} \nabla\left(\dfrac{\mu_{ec}^{m}}{T}\right) - L_{ee} \nabla\left(\dfrac{\mu_{ec}^{e}}{T}\right) - L_{e,u}\left(\dfrac{\nabla T}{T^2}\right) \\
J_u = -L_{u,m} \nabla\left(\dfrac{\mu_{ec}^{m}}{T}\right) - L_{u,e} \nabla\left(\dfrac{\mu_{ec}^{e}}{T}\right) - L_{e,m}\left(\dfrac{\nabla T}{T^2}\right)
\end{cases}
$$

$L_{i,j}$ phenomenological constant.

RELATE EACH FLUX TO ALL FORCES

VERY DIFFICULT TO SOLVE IN 3D

↓ ASSUMPTIONS TO SIMPLIFY IN CASE OF EM IN NGAP

1) $\nabla_\mu e$ ELECTROCHEMICAL POTENTIAL CAN BE NEGLECTED FOR HIGH CONDUCTIVITY MAT.

2) THERMODIFFUSION FOR GOLD ELECTRODES IGNORED

3) IN METAL WIRE FLUX of CHARGES IS DUE ONLY TO ELECTRONS

electrostatic potential

$$-\nabla\varphi = \rho \cdot j$$

ρ RESISTIVITY

j CURRENT DENSITY

$$J_m = -L_{m,m}\left(\frac{\nabla_\mu^m - z^* e \rho j}{T}\right)$$

$$Z^* = Z - \frac{L_{m,e}}{L_{m,m\,a}}$$

EFFECTIVE CHARGE

CORRECTIVE TERM DUE TO TRANFER OF MOMENTUM FROM e to IONS

$\frac{L_{m,e}}{L_{m,m}} \gg Z$ generally in EM

$\Rightarrow Z^*$ IS NEGATIVE

the NET FORCE acting on GOLD atom is in direction of electron force

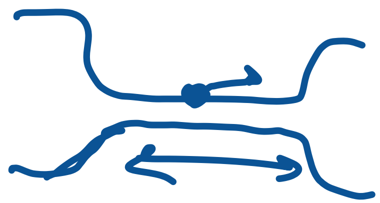
IN PRACTICE METAL ATOMS BEHAVES AS THEY HAD A CHARGE Z^* DUE TO MOMENTUM TRANSFER OF IONS

4) $$\nabla_\mu^m = \Omega \frac{\Delta\sigma}{dx}$$

FORCE due to stress σ

WIRE of L, $\Delta\sigma$ STRESS OVER LENGHT L

$$J_m = -L_{m,m}\left(\frac{\Omega \frac{\Delta\sigma}{L} - z^* e \rho j}{T}\right)$$



AS LONG AS $\Delta\sigma < \Delta\sigma_{MAX}$

EM FORCE IS BALANCED BY STRESS GRADIENT

$$J_m = 0$$

when $j \longrightarrow j_{MIN} = \dfrac{\Omega \Delta \sigma_{MAX}}{z^* \rho e L}$

↓

MINIMUM CURRENT DENSITY NEEDED TO OVERCOME STRESS AND SEE A POTENTIAL MIGRATION OF IONS

IN NORMAL CIRCUIT GIVEN A j OF A SIGNAL, A L EXISTS BELOW WHICH NO EM CAN HAPPEN

Blech's LENGHT

5) introducing $D = L^{*}_{m,m} \frac{d\mu}{dc}$ EINSTEIN RELATION

↑ DIFUSION CONSTANT

the goal is to introduce the dependency on T of the ion flow

c CONCENTRATION OF METAL IONS

μ CHEMICAL POTENTIAL

$$\mu = kT \cdot \ln c$$

↓

$$D = L^{*}_{m,m} \cdot \frac{kT}{c}$$

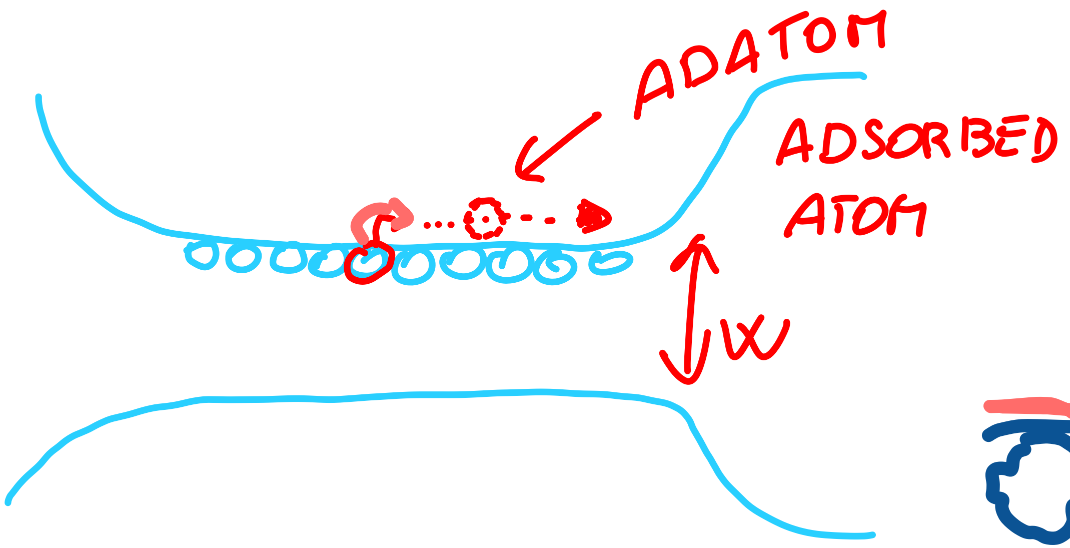
D CAN BE WRITEN ALSO AS

$$D = D_0 \cdot e^{-\frac{E_a}{KT}}$$

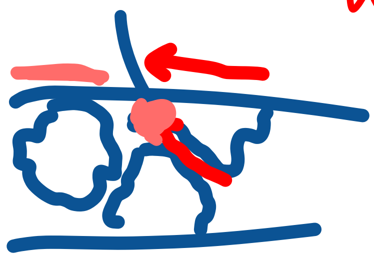
ACTIVATION ENERGY OF DIFFUSION OF IONS ON SURFACE

gold 0.12eV

IN SMALL WIRES FOR NG MIGRATION HAPENS ONLY AT THE SURFACE



NOT IN GRAIN BOUNDARIES IF $W \sim$ GRAIN SIZE



$$D = D_0 e^{-\frac{E_Q}{kT}}$$

$$D = L^{*}_{mm} \frac{kT}{C} \Rightarrow L_{m,m} = \frac{D_0}{kT} \cdot C \cdot e^{-\frac{E_Q}{T}}$$

Jm WAS

$$J_m = -L^{*}_{mm} \left(\frac{\Omega \frac{\Delta\sigma}{2} - z^{*} e \rho j}{T} \right)$$

WE OBTAINED J_{MIN} FOR MECH. STRESS

⟹ REWRITE $J_m \rightarrow f(J_{min}, T)$

$$J_m = \frac{\alpha}{T} \left(j - j_{MIN} \right) e^{-\frac{E_a}{kT}} .$$

$$\alpha = c D_0 Z^* e \rho / k$$

STRESS •

IF $j < j_{MIN} \Rightarrow J_M = \emptyset$

NO MIGRATION IF STRESS IS NOT REACHD

- TEMPERATURE

$$J_m = \frac{\alpha}{T}\left(J - J_{m_{IN}}\right) \cdot e^{-\frac{E_a}{k T_R}}$$

$$J_m = \frac{\Omega A \sigma_{MAX}}{z^* e \rho L} \qquad \alpha = c D_0 z^* e \frac{\rho}{k}$$

- FLUX OF IONS DEPENDS ON T
- GAP FORMATION STARTS AS SOON AS THE MASS FLUX IS LARGE ENOUGH
- WHEN IT HAPPENS THE LOCAL TEMPERATURE IN GAP ZONE IS INFLUENCED BY <u>JOULE HEATING</u>!

• TEMPERATURE

$$J_m = \frac{\alpha}{T}\left(J - J_{min}\right) e^{-\frac{E_a}{k T_R}}$$

$$J_m = \frac{\Omega \Delta \sigma_{MAX}}{z^* e \rho L} \qquad \alpha = C D_0 z^* e \frac{\rho}{k}$$

ONLY FOR T_{CRIT} ADATOMS ARE FORCED!

when J reaches J_{CRIT} $\neq J_{MIN}$: $T \uparrow$ NARROW WIRE $\rightarrow T_{CRIT}$ JOULE HEATING

$T > T_{CRIT}$ $\qquad p > p_{CRIT}$

$$p = \rho \cdot j^2 \qquad p_{CRIT} = \rho \cdot j^2_{CRIT}$$

→ WE NEED TO REACH T_{CRIT} FOR ION FLOW AS ADATOMS MOTION

→ WE NEED TO REACH T_{CRIT} FOR ION FLOW AS ADATOMS MOTION

→ BUT.... AS MIGRATION HAPPENS THE WIRE REDUCES

R ↗ P ↗ T ↗

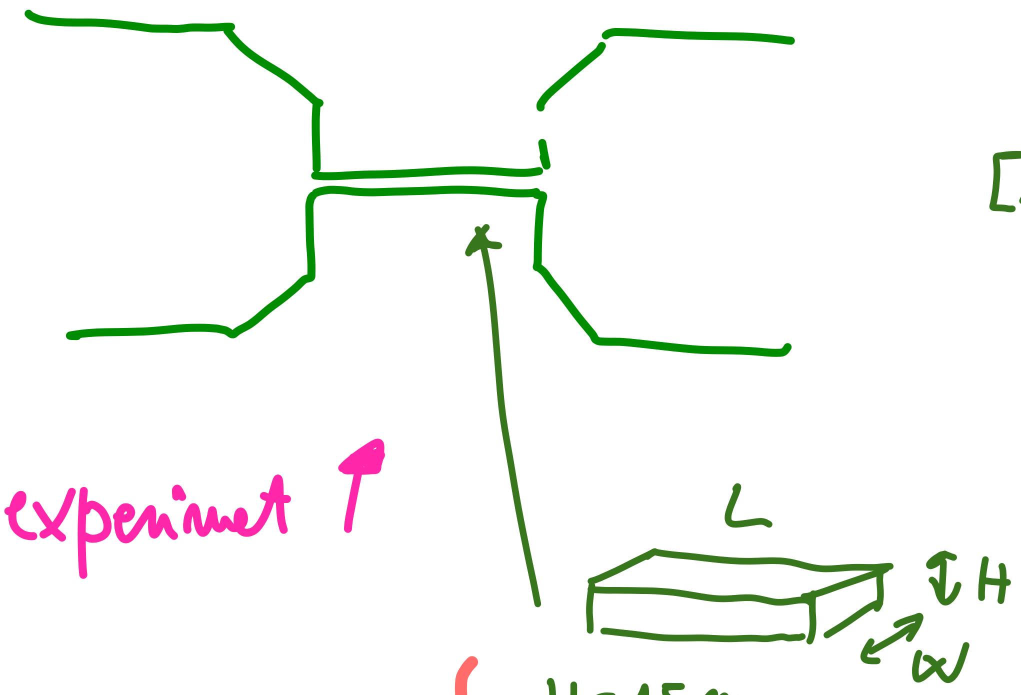
.....→ AND WHAT ?

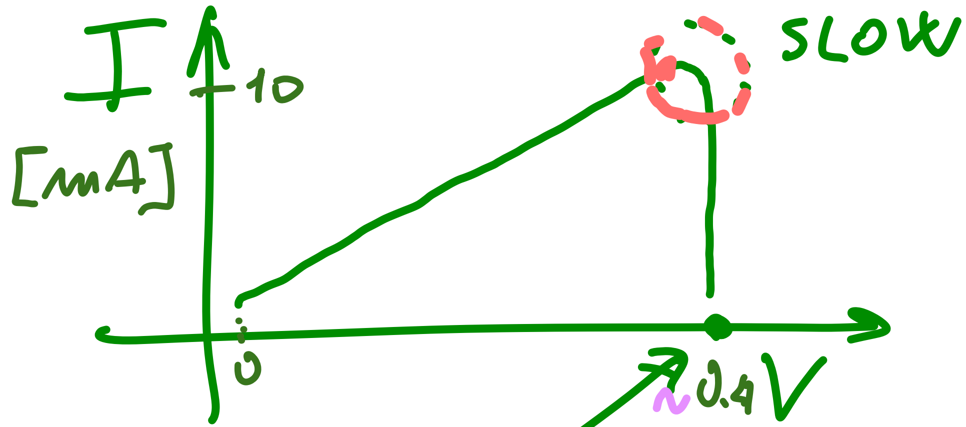
DANGER OF T. RUNAWAY

b) FAVOURING A "GOOD" EQ

When T_{CRIT} MOBILITY OF IONS INCREASES → ADATOMS
→ VACANCIES

TERRACE TYPE CONNECTION





experiment ↑

L > 1mm

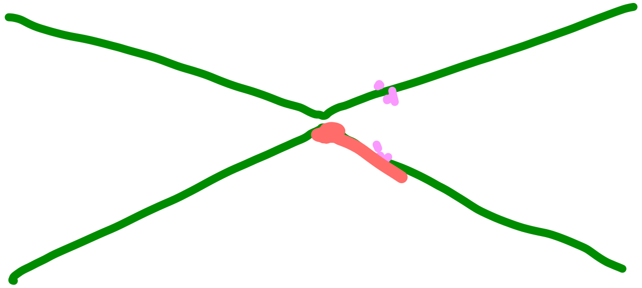
H = 15nm
W = 100nm
⊙ START

1 nm gap formed

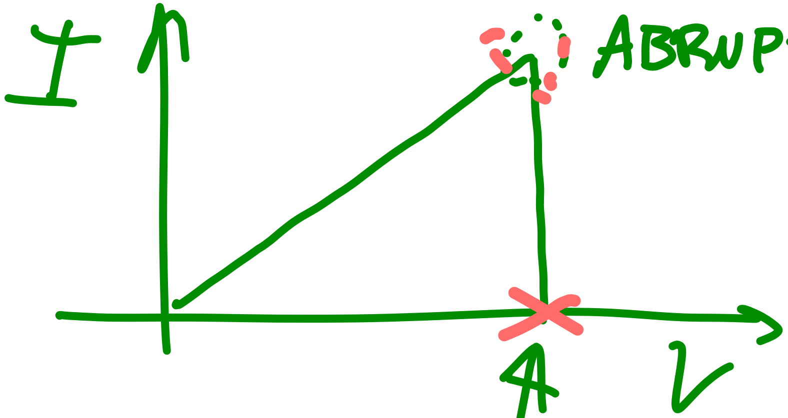
1 nA current MEASURE (TUNNEL)

WELL FORMED GAP

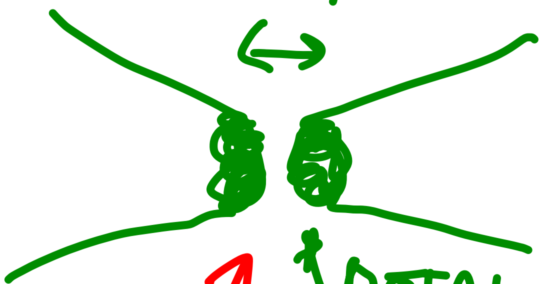
BOWE TIE TYPE



after the break



NO CURRENT



metal island

ACCUMULATION OF IONS ON GAP SIDES

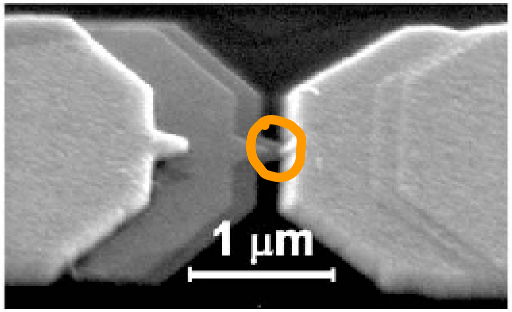
IN THIS CASE THERMAL RUNAWAY

$P \nearrow\nearrow$ $T_{LOCAL} \nearrow\nearrow$ GOLD MELTING POINT!!

NO T.R.

T.R.

(a)



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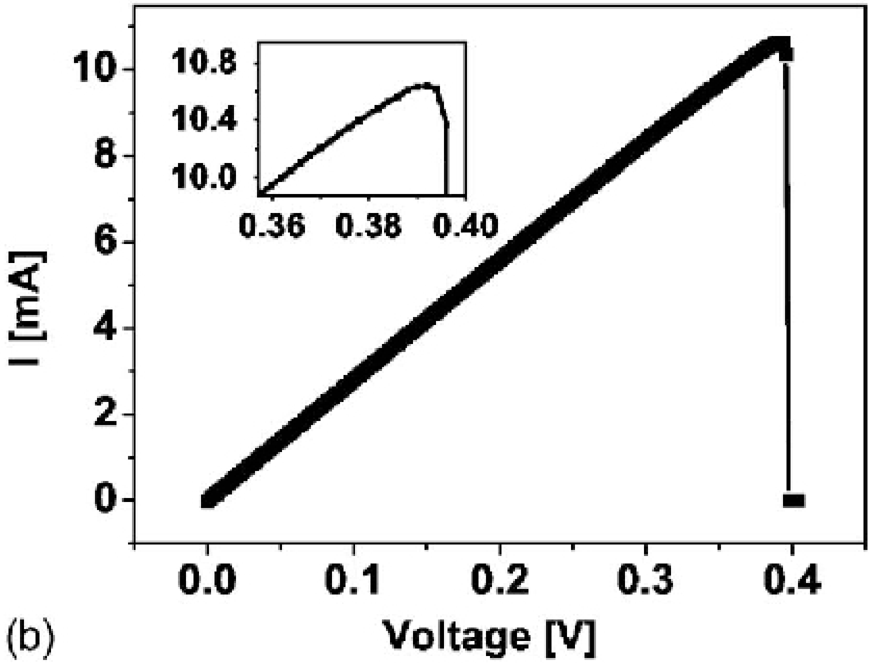
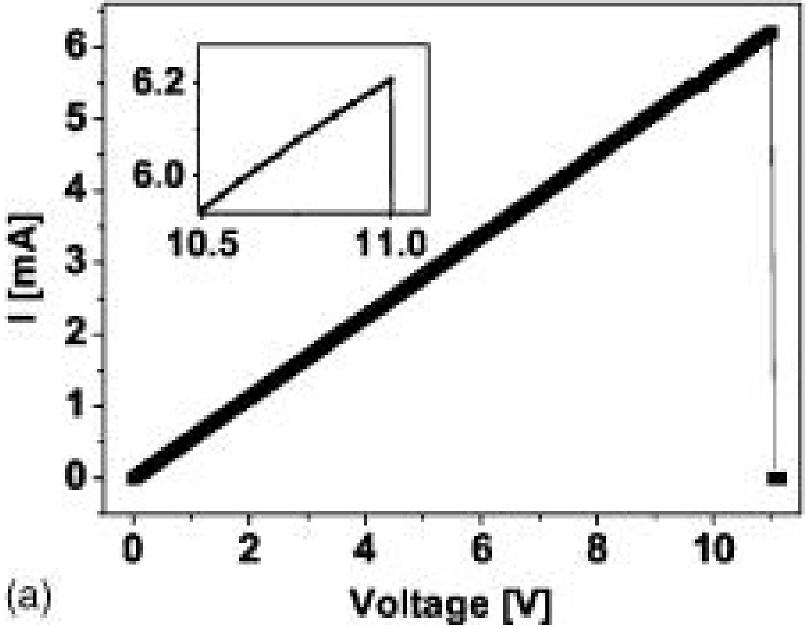


(a)



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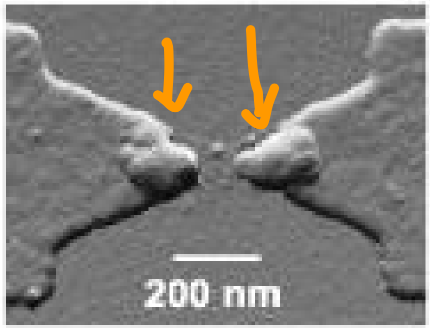
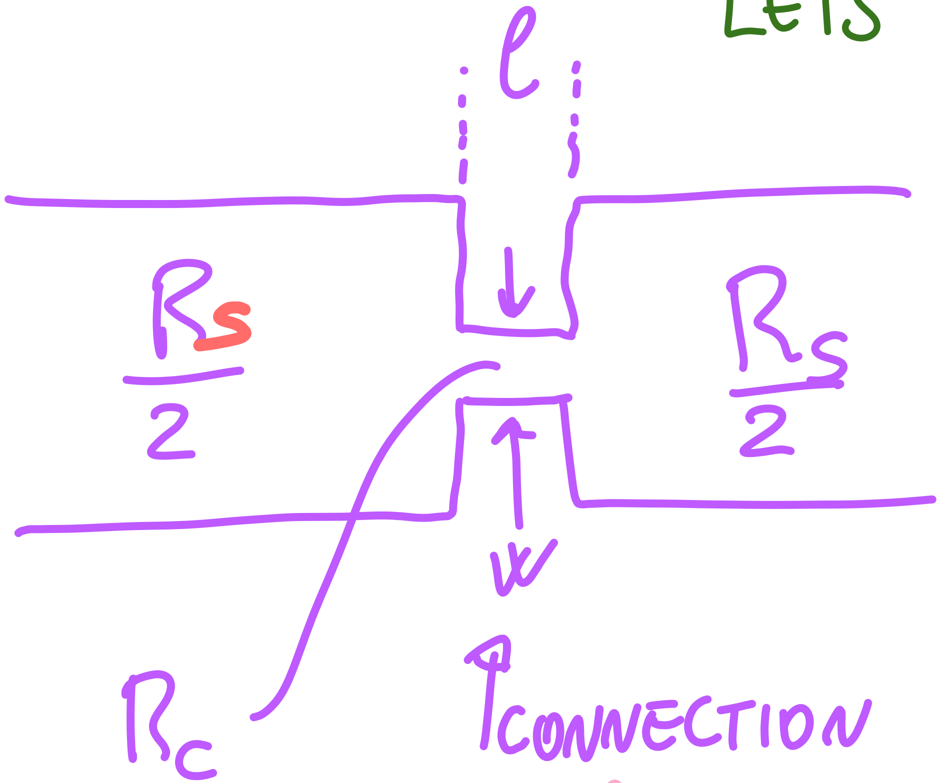


EFFECTS OF THERMAL RUNAWAY

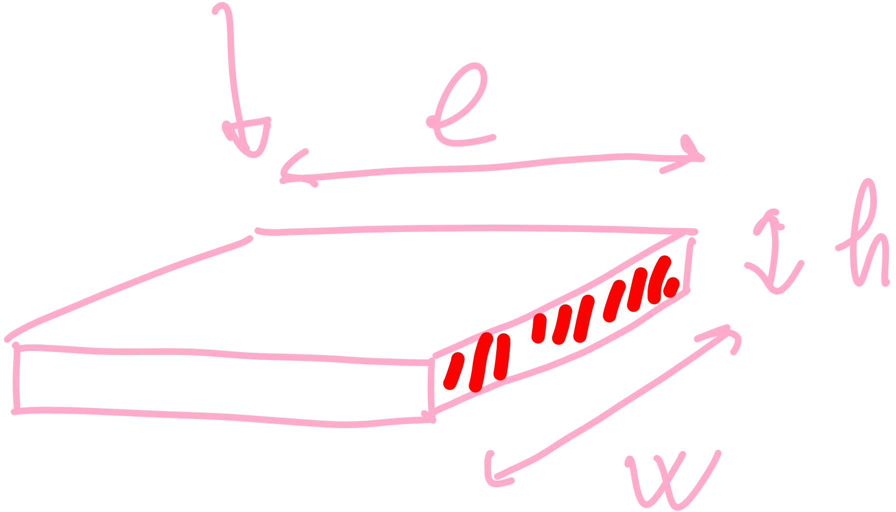
LET'S MODEL



TIME

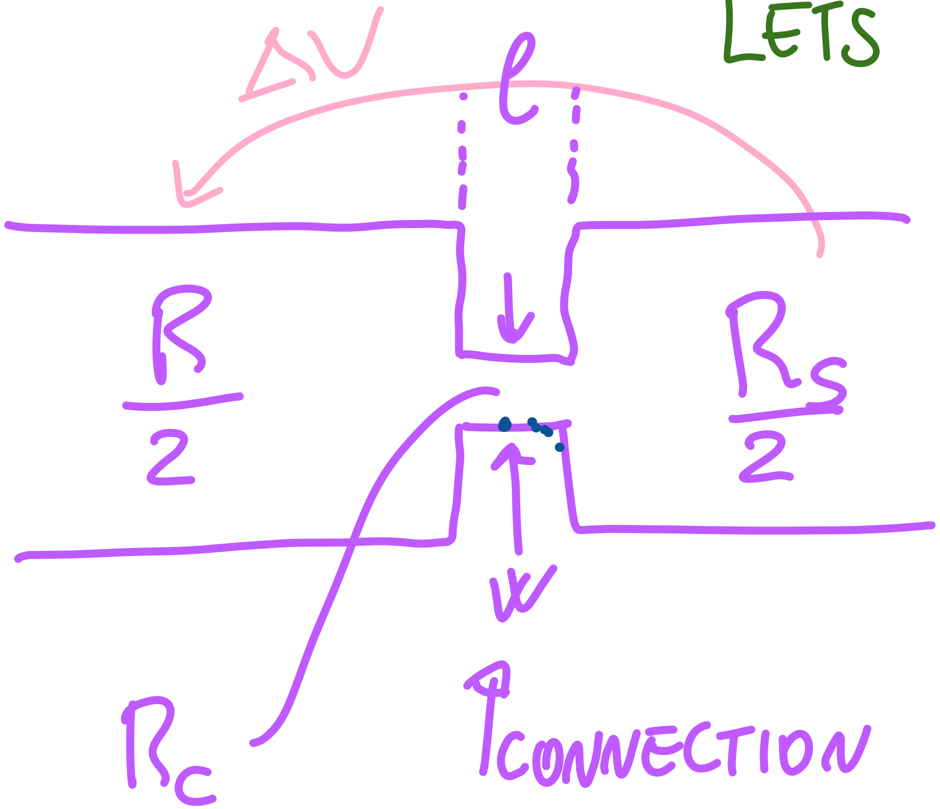
$$R_{TOT} = R_S + R_C(t)$$

$$R_C(t) = \frac{\rho\, l}{h(t)\, w(t)}$$



when MIGRATION HAPPENS h and w CHANGE IN TIME

LET'S MODEL



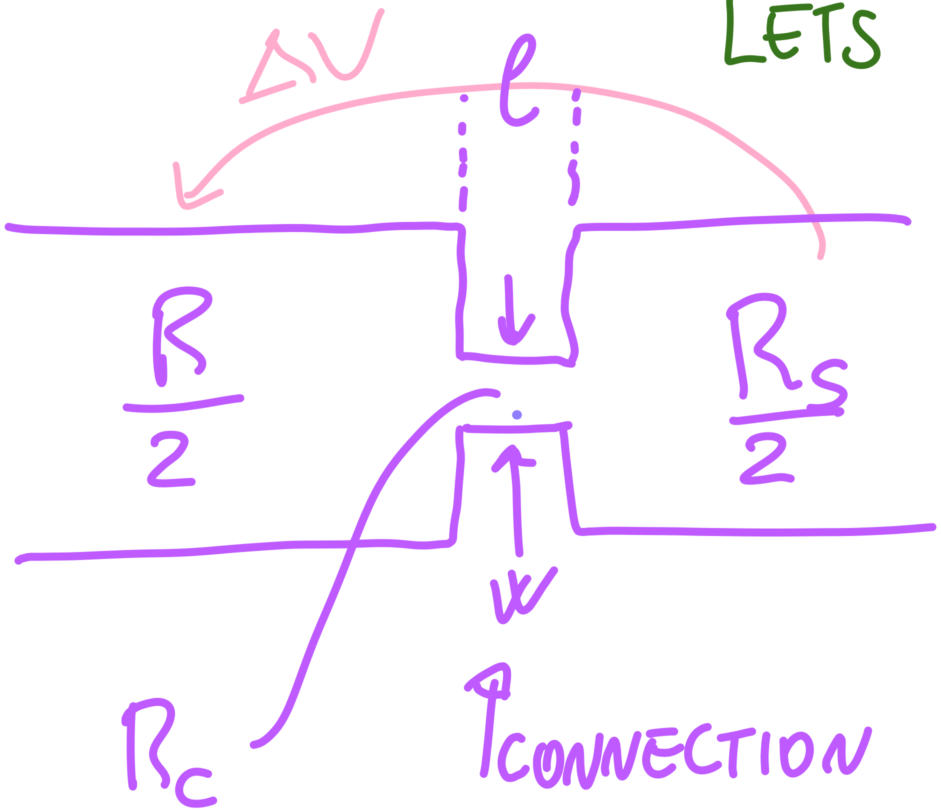
$$R_{TOT} = R_s + R_c(t)$$

$$R_c(t) = \frac{\rho \ell}{h(t)\, w(t)}$$

ΔV APPLY → J ↗ → J_{lim} Reached DUE TO STRESS

FLUX NOT NECESSARILY STARTS HERE!

LET'S MODEL



$$R_{TOT} = R_S + R_C(t)$$

$$R_C(t) = \frac{\rho \, \ell}{h(t)\, w(t)}$$

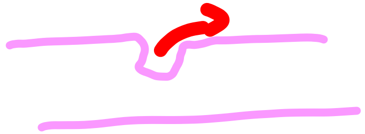
ΔV APPLY

$J \nearrow$

J_{MIN} Reached DUE TO STRESS

J STARTS WHEN FLUX, MOBILITY REACHES A VALUE due to $\underline{T}$ IN THE LOCAL POINT OF THE CONNECTION

EM STARTS → NARROW CUT (for example! 1 OR MORE)



$R_c \nearrow$ $\quad$ $p(t) \nearrow$

$$p(t) = p_{CRITIC}\left(\frac{1+\frac{R_S}{R_C(0)}}{1+\frac{R_S}{R_C(t)}}\right)^2$$

DESCRIBES INCREASE of LOCAL DISSIPATION IN CONN.

$$p_{CRIT} = \frac{V_{CRIT}^2}{\rho \ell^2} \Big/ \left(1+\frac{R_S}{R_C(0)}\right)^2$$

WHEN EM BEGINS

if $\frac{R_s}{R_c(0)} \ll 1$ SMALL STRIPES RES $p(t) \sim p_{CRIT}$

$$p(t) = p_{CRITIC} \left(\frac{1 + \frac{R_s}{R_c(0)}}{1 + \frac{R_s}{R_c(t)}} \right)^2$$

⟹ NEGLIGIBE

⟹ $p(t) \sim p_{CRIT}$ ⟹ $T \sim T_{CRIT}$

GOOD FOR "NICE" MIGRATION OF ADATOMS W/O T.R.

if $\frac{R_s}{R_c(0)} >> 1$ BIG SERIER RES $p(t) \uparrow\uparrow$ INCREASES RAPIDLY $(\ )^2$

$T|_{\text{CONNECTION POINT}}$ GRWS RAPIDLY TOWAD MELTING POINT, IONS ACCUMULATE!

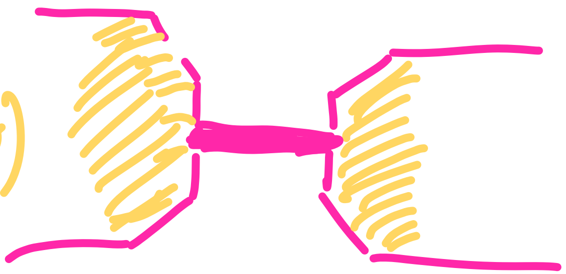
IN TERRACE TYPE

POWER REMAINS (CONSTANT) LIMITED

BECAUSE

$\frac{R_s}{R_c(0)} << 1$

$R_s << R_c(0)$



EXAMPLE $T_{CRIT.} \sim 345\,K$

in an EXP. TERRACE TYPE

$J_{MIN} \sim 4 \cdot 10^{8}\ \frac{A}{cm^2}$ for good

BUT

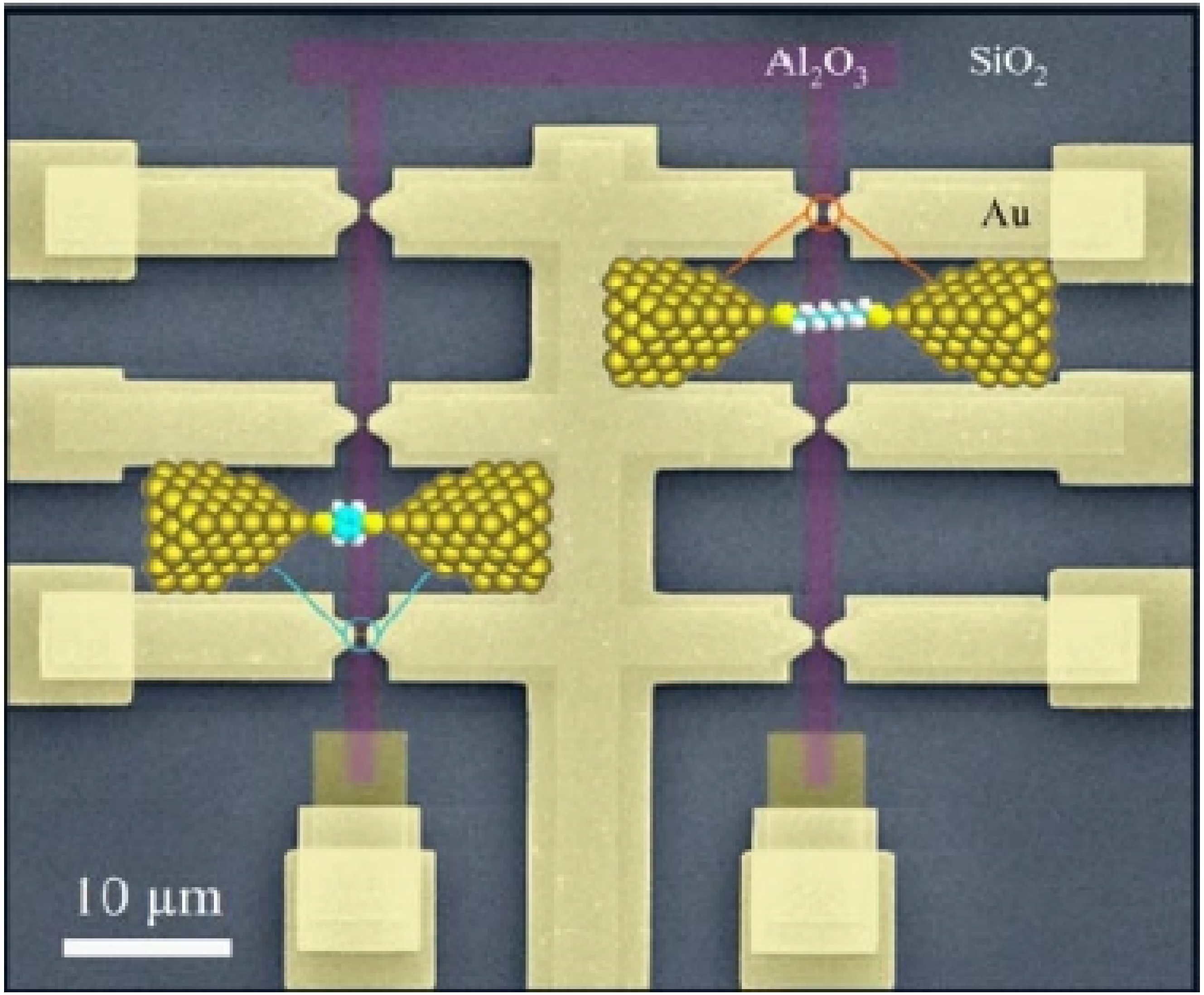
if TEMP. 295 K → T → 4.2 K

$J_{CRITICAL}$ ↗ 50% HAS TO RISE TO

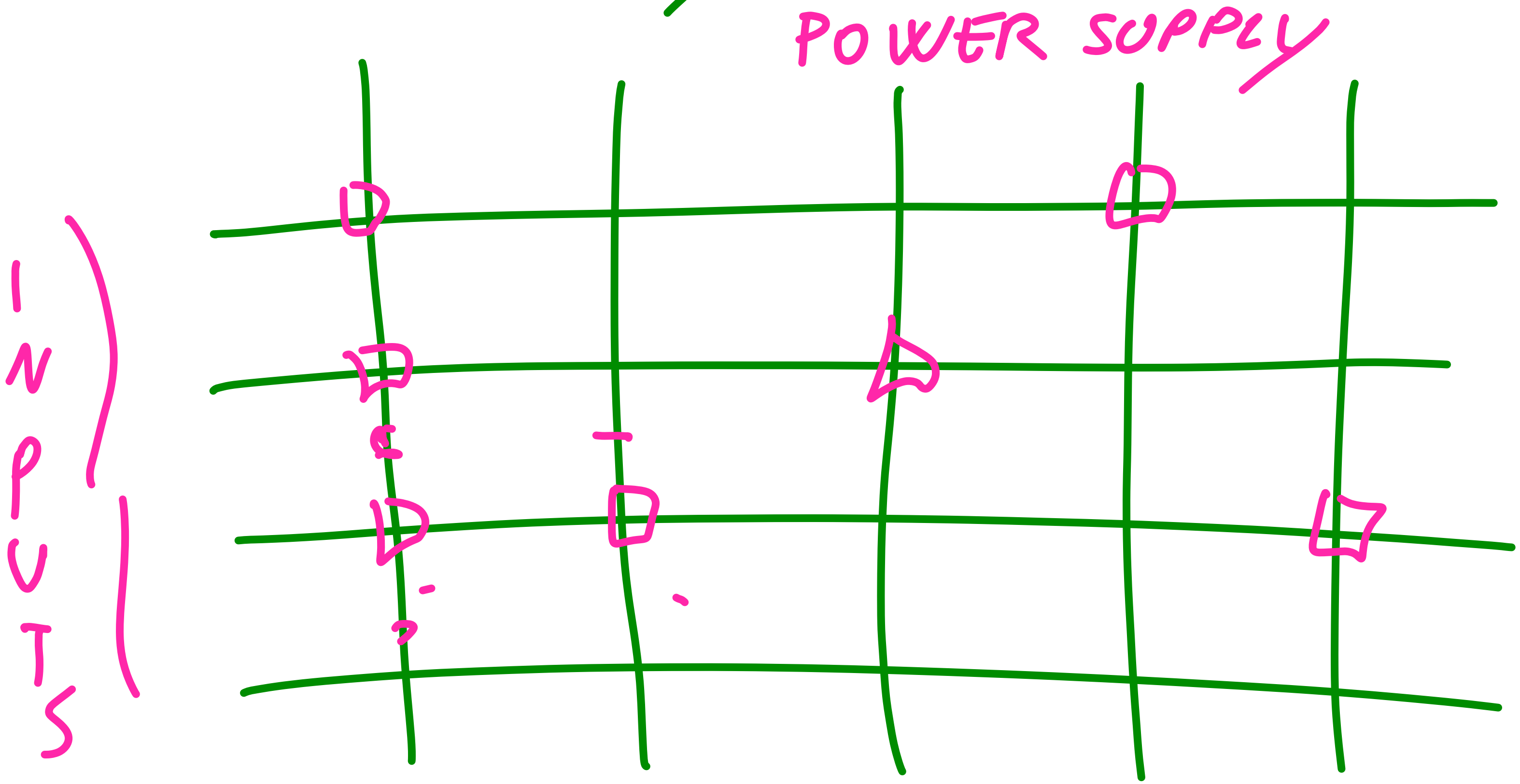
to reach $P_{CRIT.}$

T_{CRIT}

c) N.G. ARRAYS BASED ON N.G.



IN A SYSTEM WE EXPECT

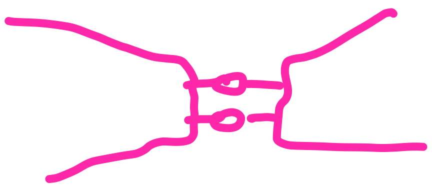


MATRIX OF WIRES OF M.T CONNECTED // OR SERIES

→ LOGIC! FUNCTION

P.L.A → FPGA

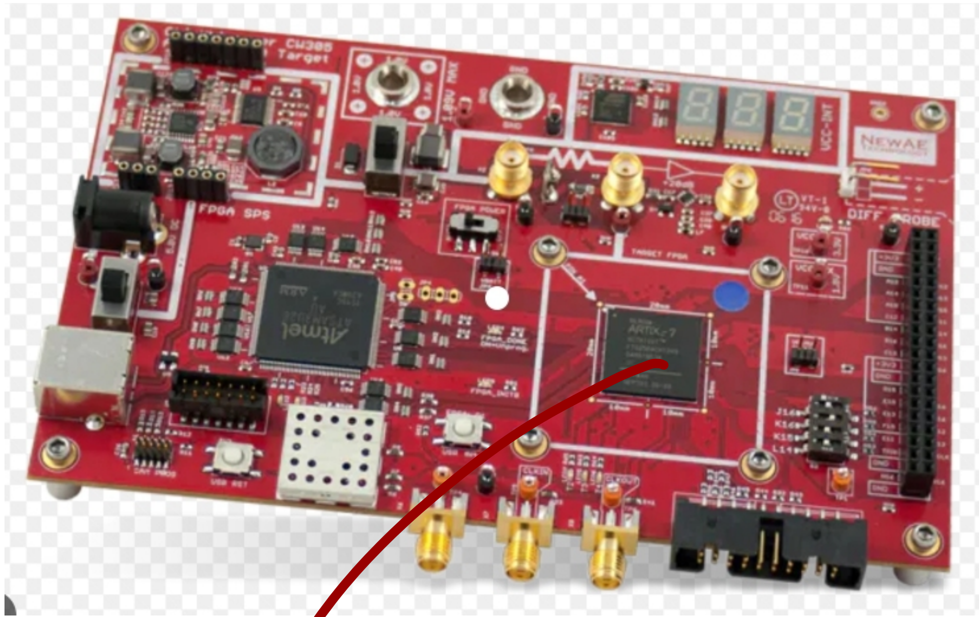
IN CONVENTIONAL TECH

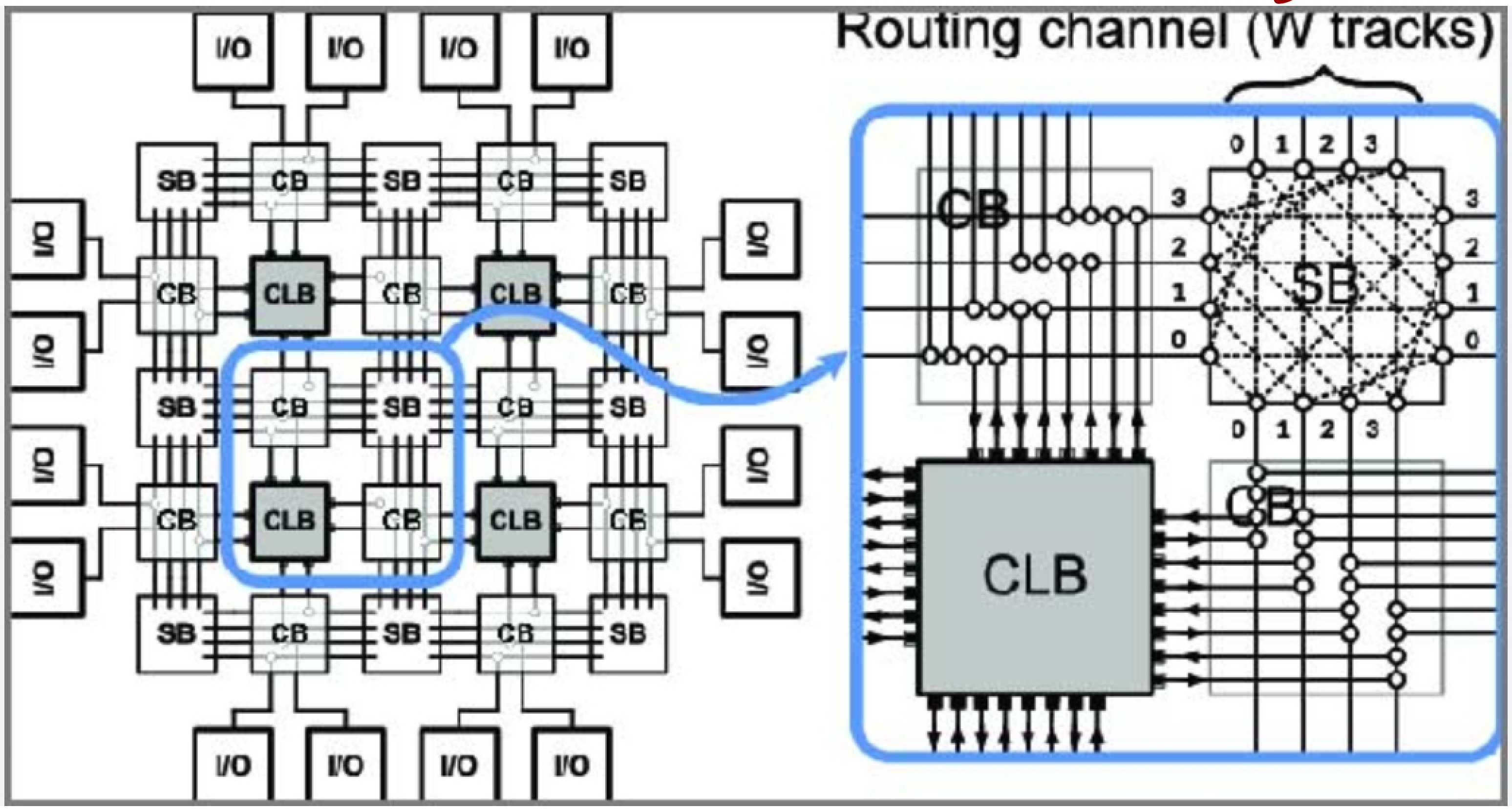


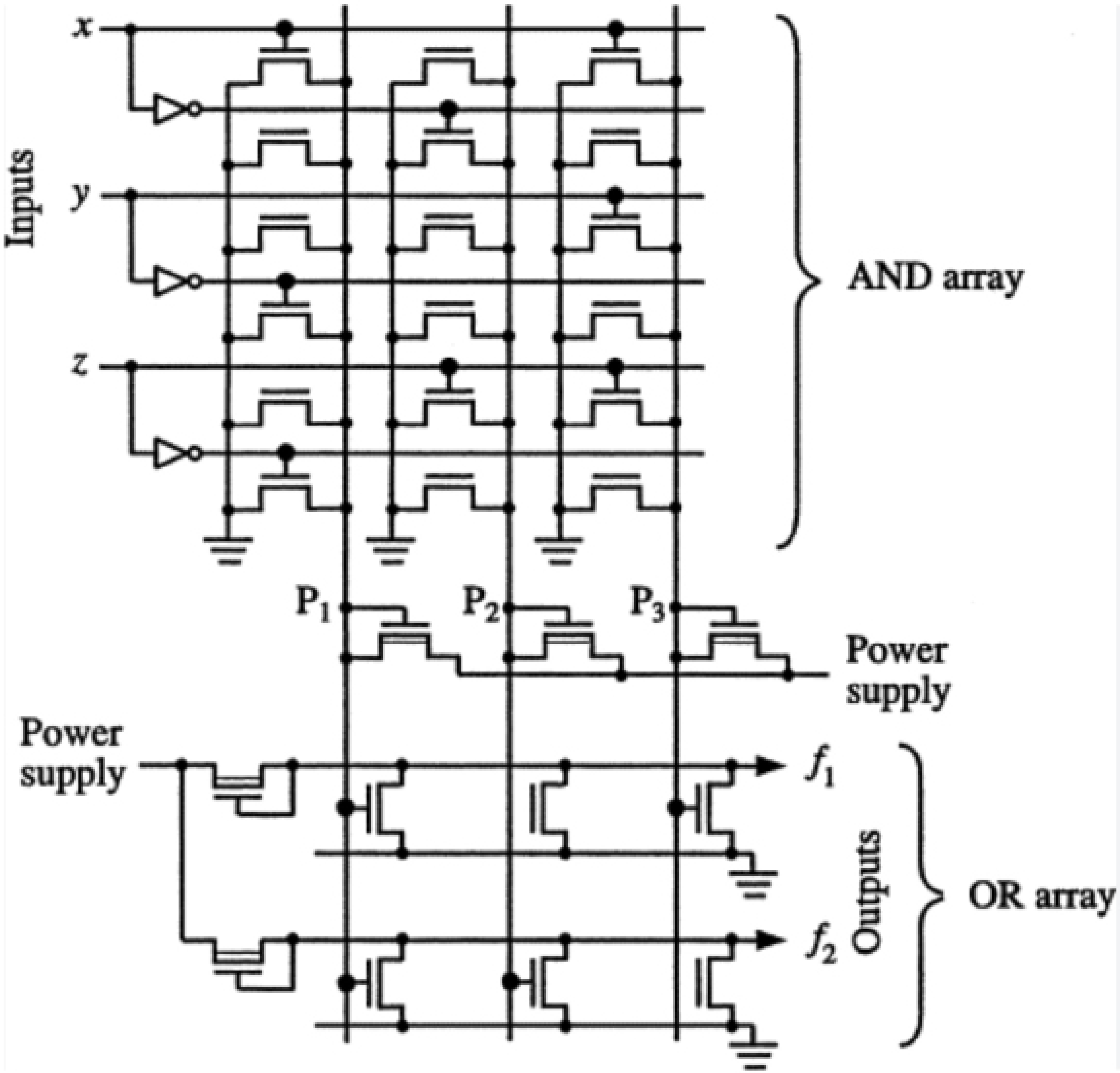
FABRICATION OF ARRAY OF NGAPS IS NEEDED!

MODERN FPGA

FIELD PROGRAMMABLE GATE ARRAY







FORMER PLA

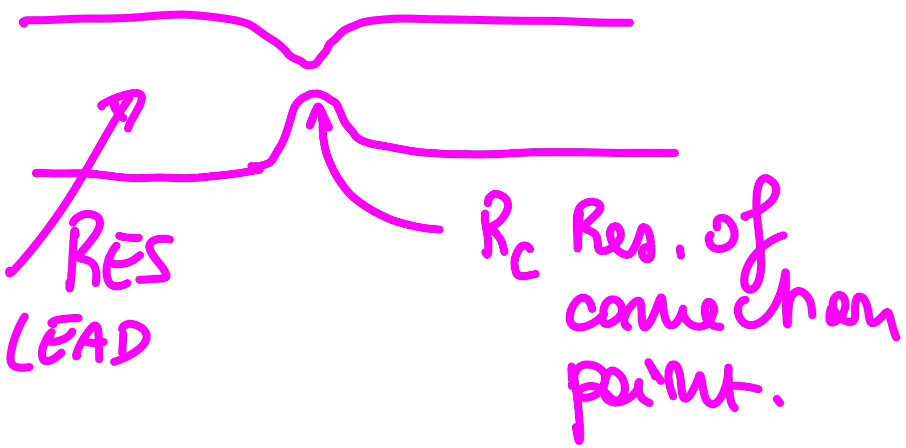
PROGRAMMABLE LOGIC ARRAY

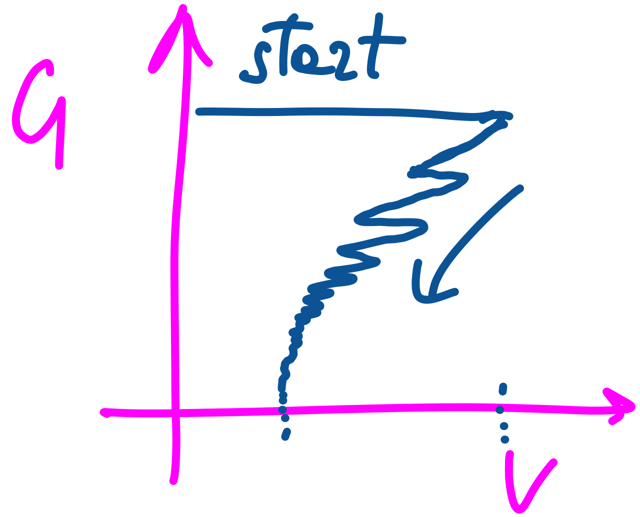
WHEN TECH WAS LESS RELIABLE AND EVOLVED

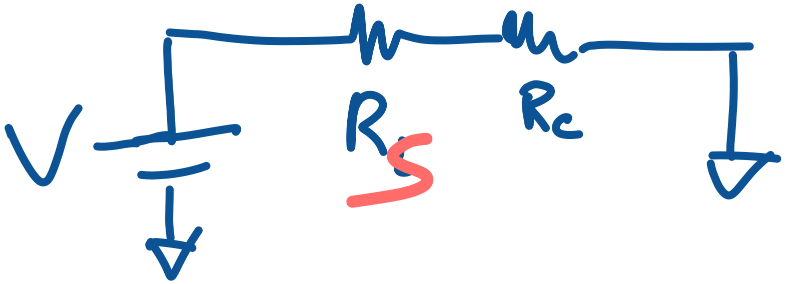
REGULARITY HELPS!!

PARALLEL FABRICATION OF NGAP via FCE

CASE (A) 1 DEVICE







FCE ADJUSTS V so that power at junction

$P > P_{CRITICAL}$

$P <$ MELTING POINT

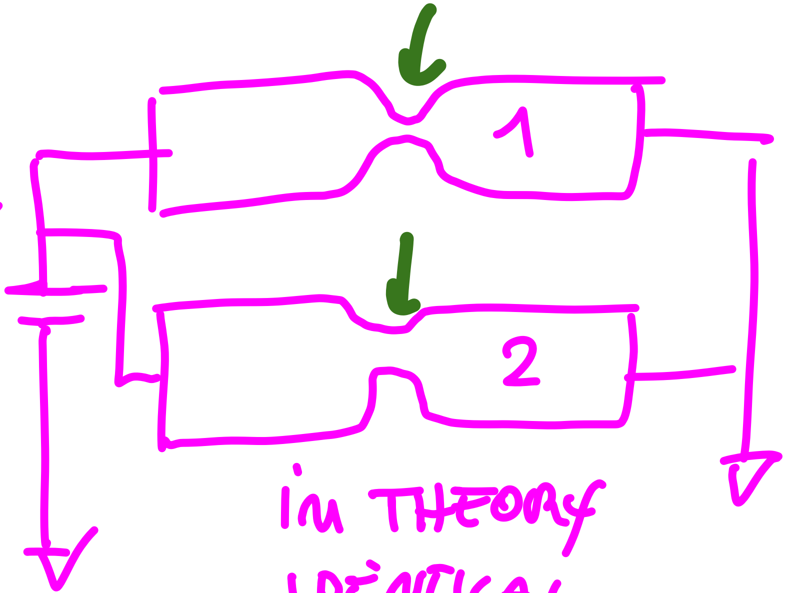
SEVERAL STEPS UNTIL

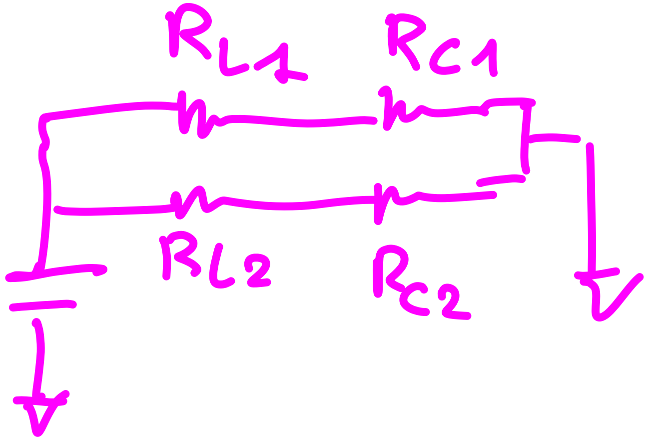
$R_c \sim 4k\Omega$

FINAL LIMIT BEFORE BREAK

CASE (B)

2 DEVICES SEPARATED CONTROLLED in //





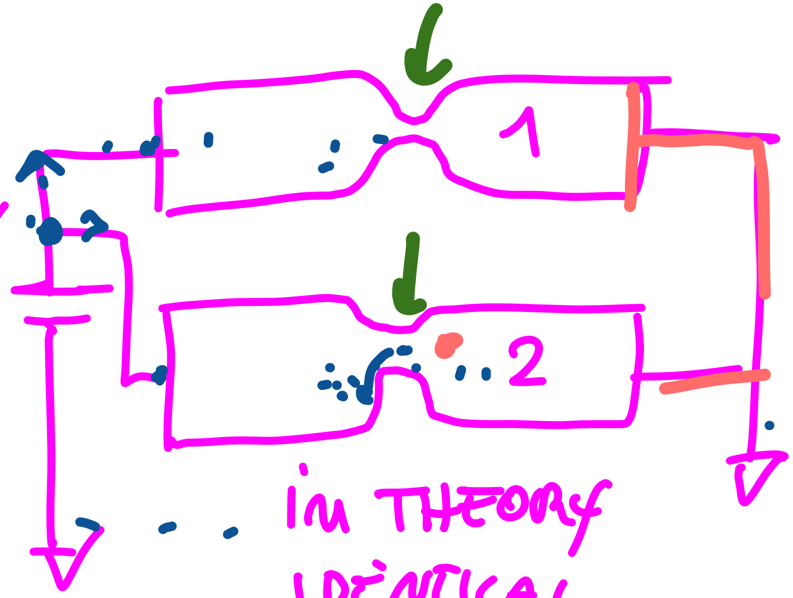
in THEORY IDENTICAL

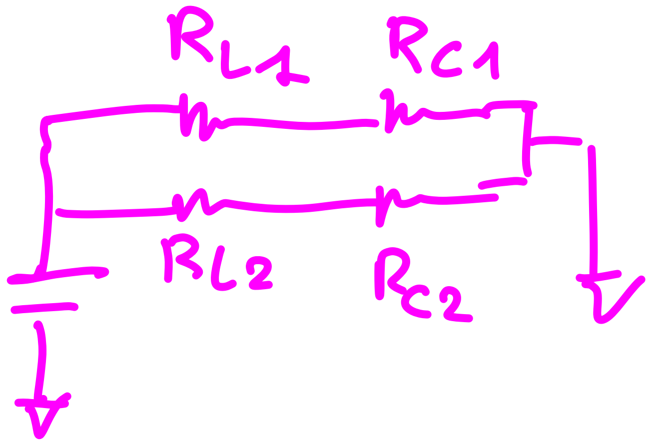
$R_{L1} = R_{L2}$ $R_{C1} = R_{C2}$

WE EXPECT THEY BEHAVE IN THE SAME WAY

CASE (B)

2 DEVICES SEPARATED CONTROLLED in //

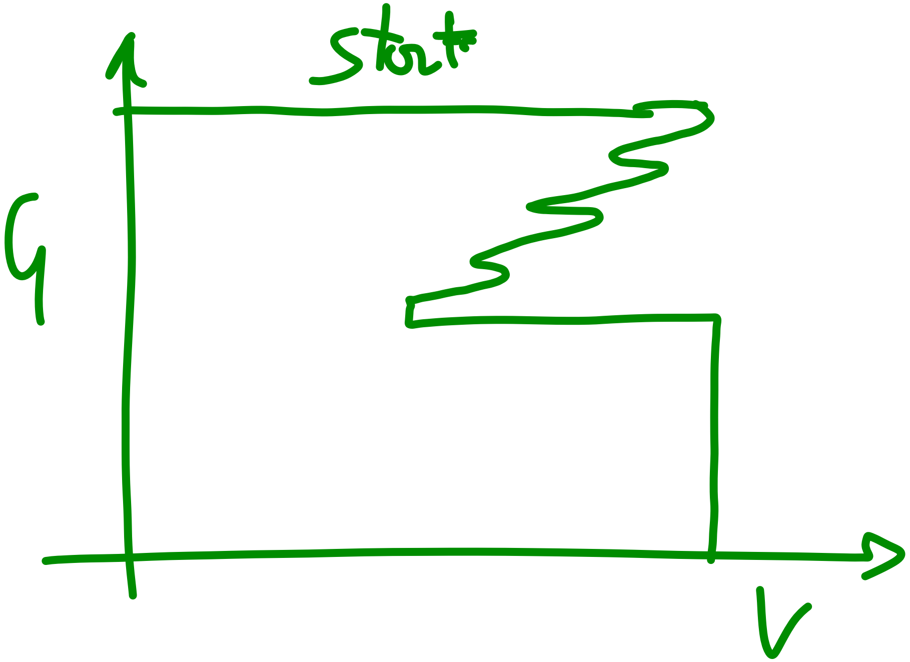




in THEORY IDENTICAL

WE EXPECT THEY BEHAVE IN THE SAME WAY

$R_{L1} = R_{L2}$ $R_{J1} = R_{J2}$



RESULT: 1 GAP IS OK

THE SECOND HAS BUMPS, BIGGER ...!

THERMAL RUNAWAY TRIGGERING REACHED!

PROCESS VARIATIONS !

$R_{C1} \neq R_{C2}$

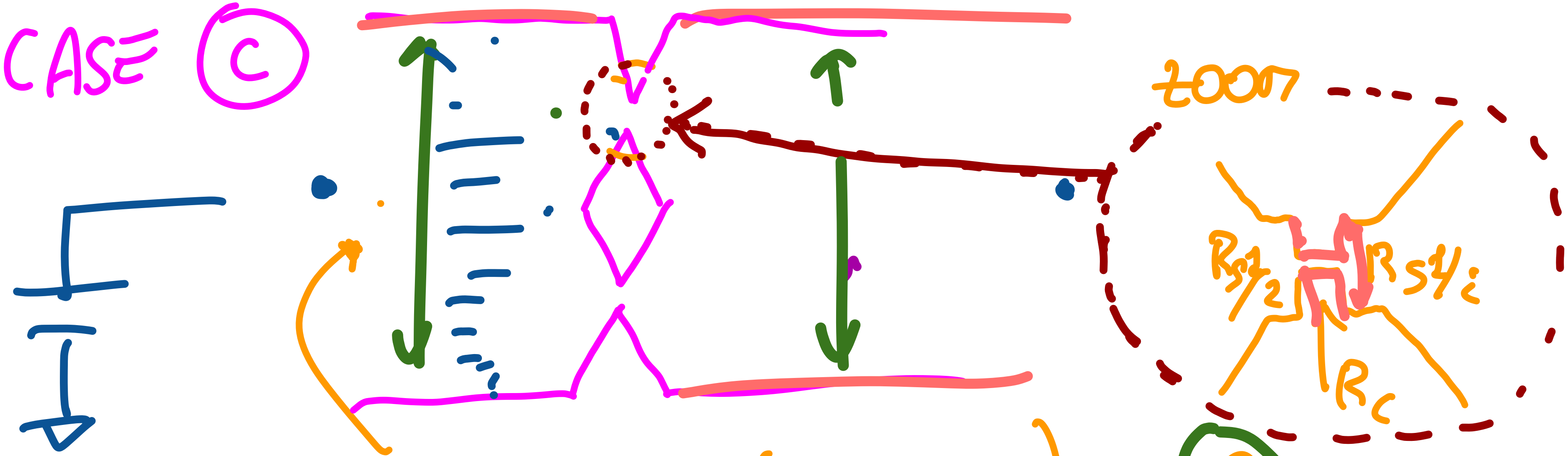
ex. $R_{C1} \sim 4.2\,\Omega$ $R_{C2} \sim 4\,\Omega$

AFTER A WHILE R_{C1} ↑ WILL BREAK AT FIRST BECAUSE IT REFLECTS A SMALLER WIRE, SO IT IS CONSUMED FIRST: AS SOOS AS IT BREAKS

→ ALL CURRENT GOES SUDDENDLY IN THE SECOND CONNECTION

→ MELTING WILL BE THE RESULT

CASE (C)



$$R_{TOT} = R_L + R_S + (R_{c1} // R_{c2})$$

(R_S: TOTAL SAMPLE)

R_S HAS TO BE WELL DESIGNED W.R.C. R_C

if $R_s < R_{c1}, R_{c2}$ then

even if for ex. $R_{c1} > R_{c2}$ DUE TO P. VARIATION

$\frac{\partial P_1}{\partial R_{c1}} < \frac{\partial P_2}{\partial R_2}$

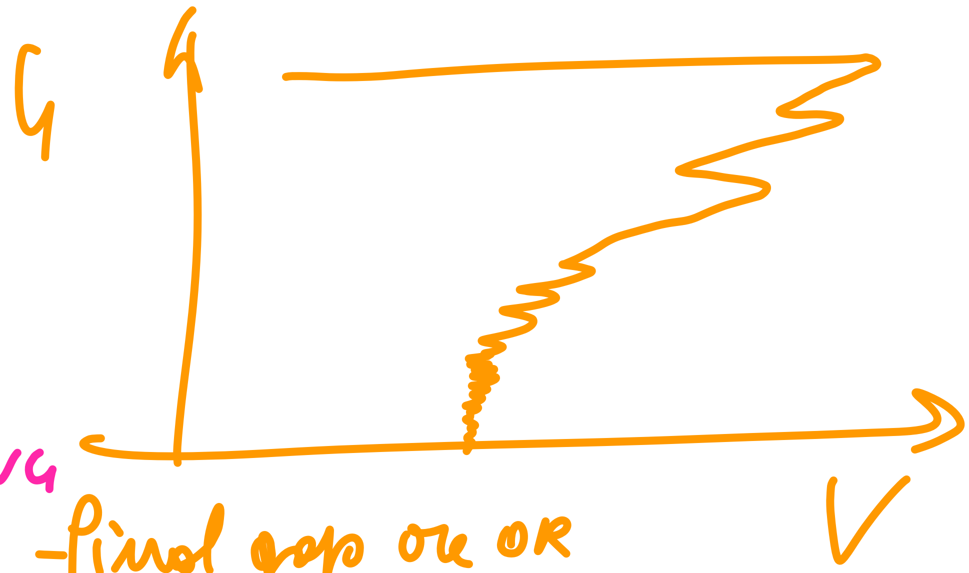
↓

CURRENT GOES TO OTHER CONNECTION

P_c INCREASE

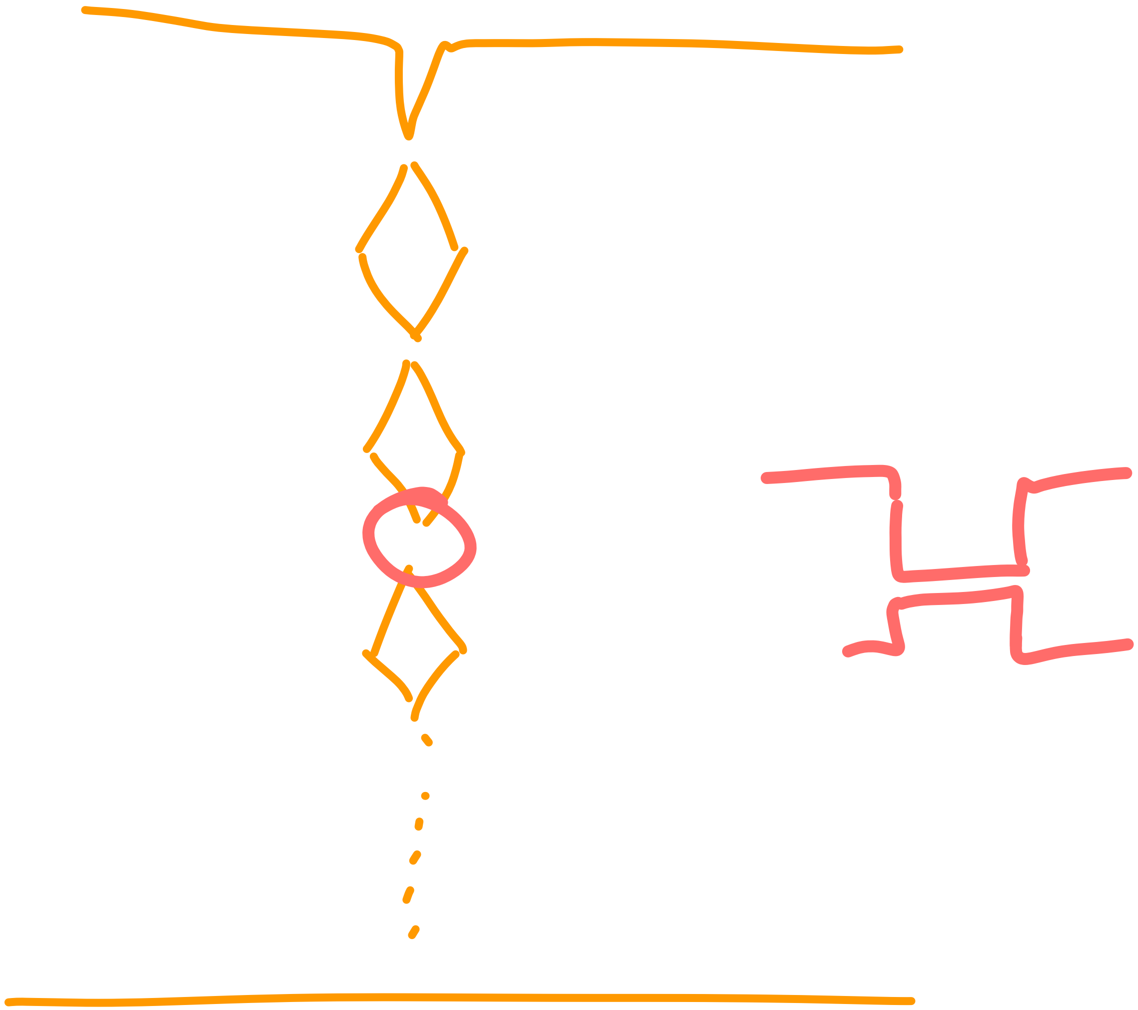
GAPS ARE GENERATED ALMOST AT THE SAME TIME

POWER DUE TO SELF HEATING REMAINS IN PCRIT EVEN IF 1 CONN. BREAKS



final gap or OR

SAME THING WITH SEVERAL CONNECTION IN PARALLEL



⇒ IT WORKS WELL UP TO A CERTAIN NUMBER OF ELEMENT

⇒ REQUIRES CAREFUL CONTROL & WIRING

CRISTALLIZATION

a) EM PHYSICAL MODELLING

b) FOVOURING A GOOD EM

c) ARRAYNG. WITH EM