

# Моделирование отказов элементов металлизации микро- и наноэлектронных устройств под действием электромиграции

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**Key problems in failure modeling are to model**

- (i) vacancy/ion transfer and accumulation, and**
- (ii) defect nucleation and growth induced by these processes**

**This work presents a full 3D theory and the results of a computer simulation of electromigration-induced nano- and microprocesses that terminate in failure of thin-film conducting elements. These processes determine operational reliability and lifetime of IC metallization**

## Empirical relation of Black (1969)

$$\text{TTF} = A j^{-n} \exp\left(\frac{E_a}{kT}\right)$$

$j$  is the current density,

$E_a$  is the activation energy of grain boundary diffusion,

$A$  is the parameter depending on the material, process of line formation, conductor structure and geometry,

$n \geq 1$  is the constant whose value essentially depends on the range of the  $j$  values used ( $n$  increases with  $j$  growth)

T. Makhviladze, M. Sarychev, and K. Valiev (1989) -  
microscopic theory

T. Makhviladze, M. Sarychev, and K. Valiev (1990 - 1991) -  
more general model

# THEORY OF ELECTROMIGRATION DEGRADATION AND FAILURES (MAIN EQUATIONS)

## VACANCY TRANSPORT AND STRESS GENERATION

$$\frac{\partial C}{\partial t} + \nabla_i q_i = F_v(x_1, x_2, x_3, t), \quad q_i = D \left( -\nabla_i C + \frac{C Z^*}{k T \sigma_0} j_i + \frac{C}{k T} \varepsilon_v \frac{\partial \sigma}{\partial x_i} \right)$$

$C(x_1, x_2, x_3, t)$  is the vacancy concentration,

$q_i$  is the  $i$ -th component of the diffusion flow,

$F_v(x_1, x_2, x_3, t)$  is the source function describing vacancy generation and annihilation,

$D$  is the vacancy diffusion coefficient,

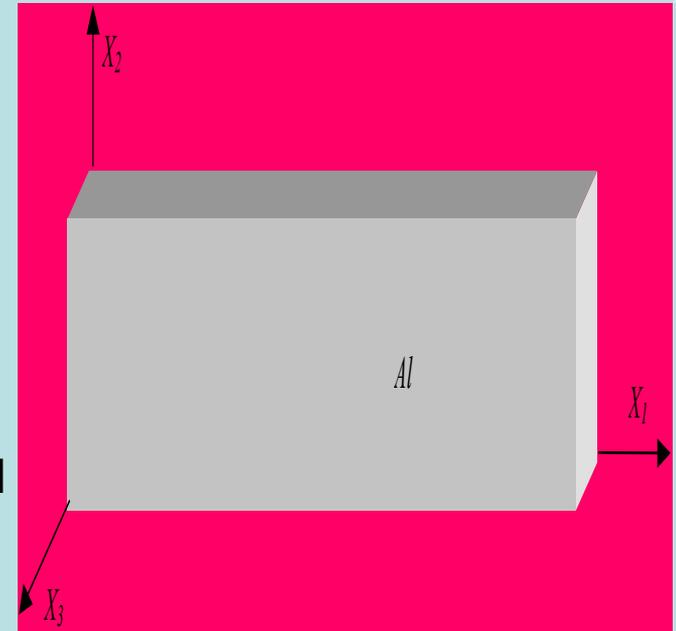
$Z^*$  is the effective vacancy charge,

$j(x_1, x_2, x_3)$  is the current density vector,

$\sigma(x_1, x_2, x_3, t) = (\sigma_{11} + \sigma_{22} + \sigma_{33}) / 3$  is the spherical component  $\sigma$  of the mechanical stress tensor  $\sigma_{ij}$  which describes triaxial compression,

$\varepsilon_v$  is the elastic volume strain induced by the relaxation of the vacancy volume ( $\varepsilon_v = -f \Omega < 0$  with the relaxation coefficient  $f$ ,  $\Omega$  is the specific atomic volume of the conducting material),

$\sigma_0$  is the conductivity



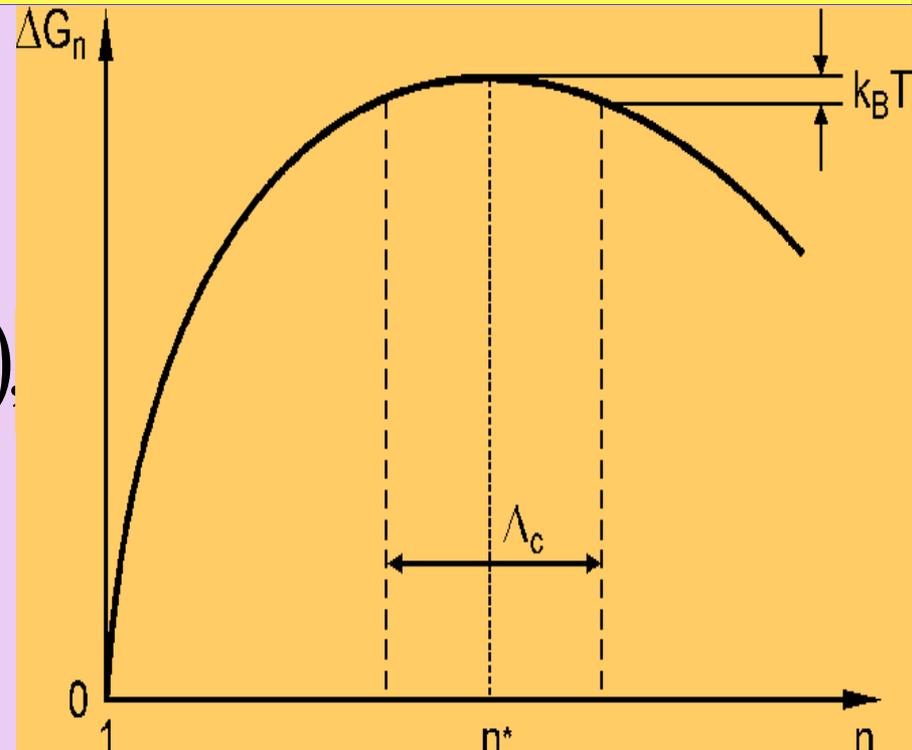
# VACANCY CLUSTER NUCLEATION KINETICS AND DETERMINATION OF THE MICROVOID NUCLEATION TIME

The equilibrium concentration of vacancy clusters of size  $n$  is

$$c_0(n) = c_0(1) \exp(-\Delta G_n / kT)$$

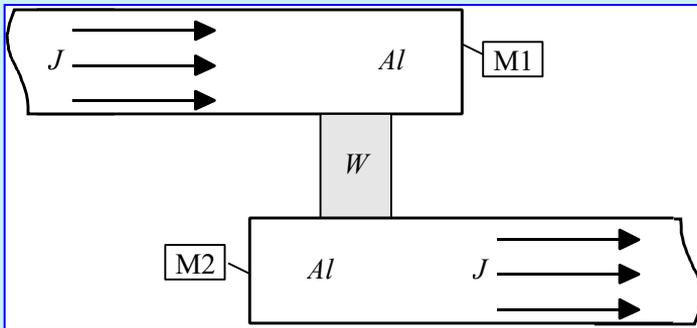
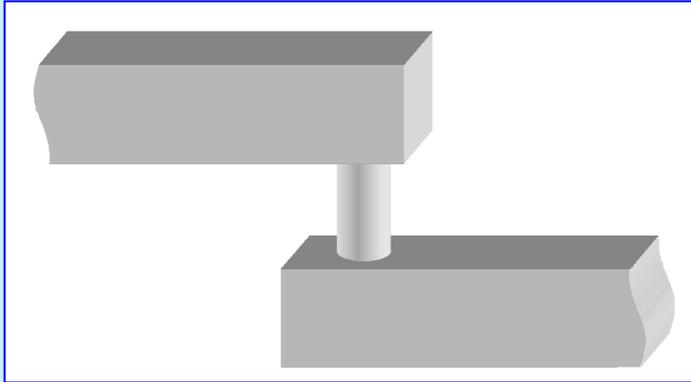
where  $c_0(1)$  is the equilibrium concentration of vacancies,

$\Delta G_n$  is the change in Gibbs free energy resulting from the formation of a vacancy cluster of size  $n$ .

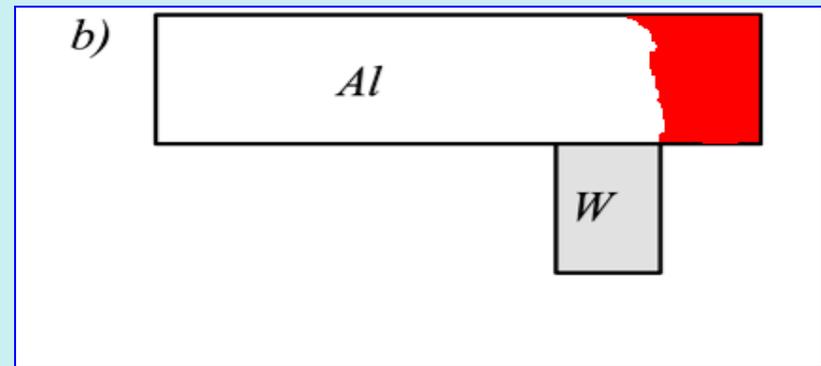
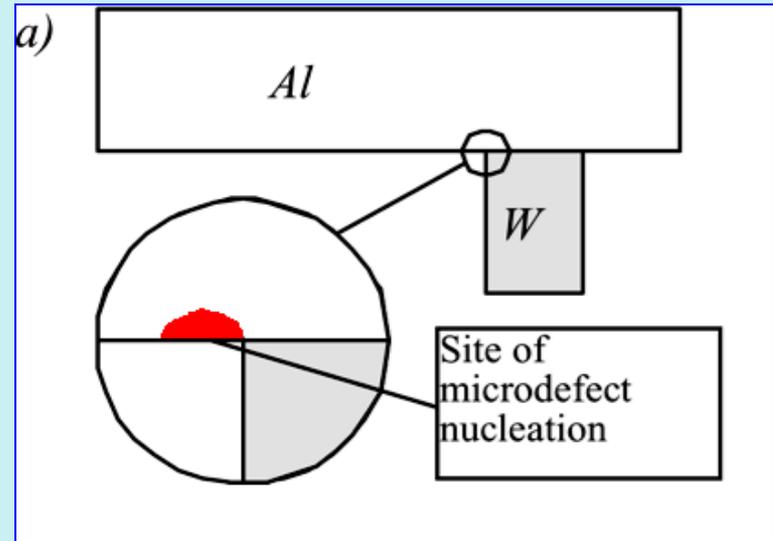


Qualitative relationship between Gibbs free energy variation and cluster size.  $\Delta n_c$  is the width of the domain on the size axis where the free energy variation differs by no more than  $k_B T$  from its maximum value

# MULTILEVEL-METALLIZATION DEGRADATION AND FAILURE

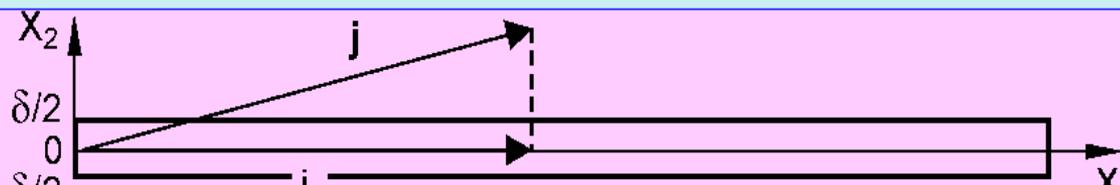
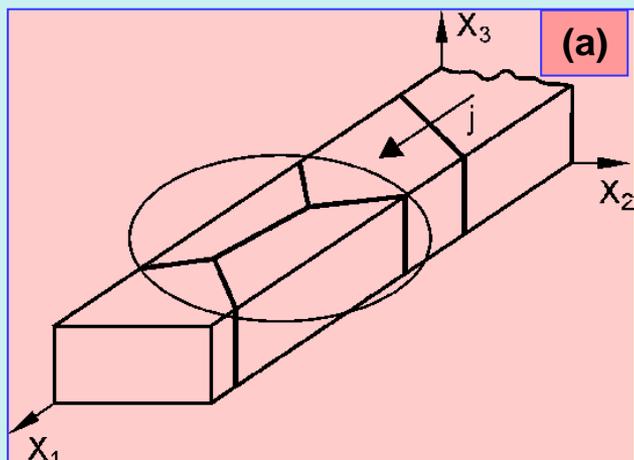


**Two-level metallization with the AL conducting lines interconnected by a tungsten via**

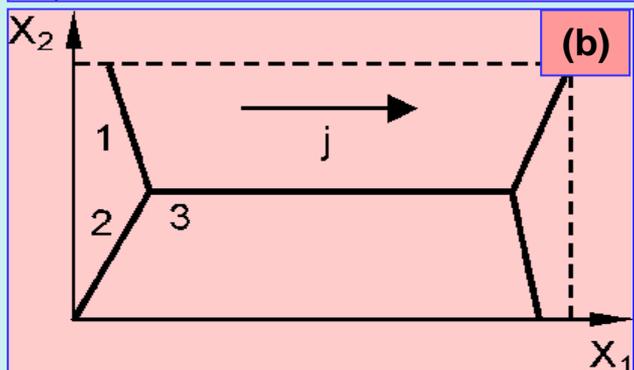


**Two possible mechanisms of metallization failure: (a) voiding and (b) surface erosion**

# POLYCRYSTALLINE INTERCONNECT DEGRADATION AND BULK FAILURE



Frame of reference relative to a rectilinear grain boundary part.  $\delta$  is the grain boundary width,  $j_1$  is the projection of the current density vector on the  $X_1$  axis



Conducting line (substrate and coating not depicted) (a); top view of the line segment under study (the digits denote rectilinear parts of the grain boundary converging in the triple point) (b)

## The used values of parameters

Bulk modulus  $B = 60$  GPa,

$\rho_0 = 3 \cdot 10^{-8}$  Ohm  $\cdot$  m

Effective vacancy charge  $Z^* = 12|e|$  ( $e$  is the electron charge),

Activation energy of grain-boundary diffusion

$E_a^{GB} = 0.6$  eV,

Activation energy of bulk diffusion  $E_a^B = 1.2$  eV,

$f = 0.2$ ,

Interatomic distance  $a = 2.5 \cdot 10^{-10}$  m,

Volume of a unit cell  $\Omega = 1.66 \cdot 10^{-29}$  m<sup>3</sup>,

Grain boundary width  $\delta = 0.5$  nm

Segment length 2 mkm

# Cu metallization degradation: Problems and Features

- **Failure kinetics: vacancy electromigration, generation of mechanical stress and deformation, nucleation and growth of vacancy clusters ( $j > 10^5 - 10^6$  A/cm<sup>2</sup>)**
- **Growth of thermodynamically stable microvoids from nanometer size up to transverse size of the line (up to grain size, for bamboo structures)**
- **Competition of different electromigration failure modes in the contact areas of conducting lines:**
  - 1) microvoid growth in the vicinity of contact plug connections between the adjacent metallization levels
  - 2) open edge erosion of the conducting line as a result of vacancy migration to the open end of a line

**The other failure modes:**

  - 3) microvoid growth at the line - isolating dielectric interface (deep into the line bulk)
  - 4) microvoid growth in the bulk of polycrystalline line due to grain boundaries electromigration and stable cluster nucleation in the triple points (less important for Cu compared with Al)

- **Adhesion strength of interfaces subjected to the action of electrical, mechanical and thermal load and its dependence on defectiveness of joining materials (no exfoliation, hogging etc.)**  
**Interfaces and contacts: conducting line (CL) - barrier film layer, CL – protective dielectric, CL – layer introduced between CL and plug to improve adhesive power (Ta, TaN, TiN); metal electrodes - high-K dielectric – high mobility semiconductors**
- **Optimization of interconnect adhesion strength with respect to defect concentrations and distributions, boundary texture, and operating parameters**
- **Resistivity increase and heating due to the need for barrier film (up to 20% of the wire width) to prevent Cu from diffusing into the surrounding dielectric**
- **Theory and modeling problems concerning Cu metallization**  
**it is necessary further development of microscopic discrete theory of vacancy and ion transport as well as deformation processes, atomistic description of conducting component structure**

### **Публикации:**

- **Т.М.Махвиладзе, М.Е.Сарычев.** Теория электромиграционной неустойчивости границы соединенных проводящих материалов // Труды Фтиан. 2018. Т.27. С.97-104.
- **Т.М. Махвиладзе, М.Е. Сарычев.** Теория электромиграционных отказов межсоединений с учетом диффузии френкелевских пар // Труды ФТИАН. 2019. Т.28. С.20-31.