# GRAIN BOUNDARY STRUCTURE and DEFECTS

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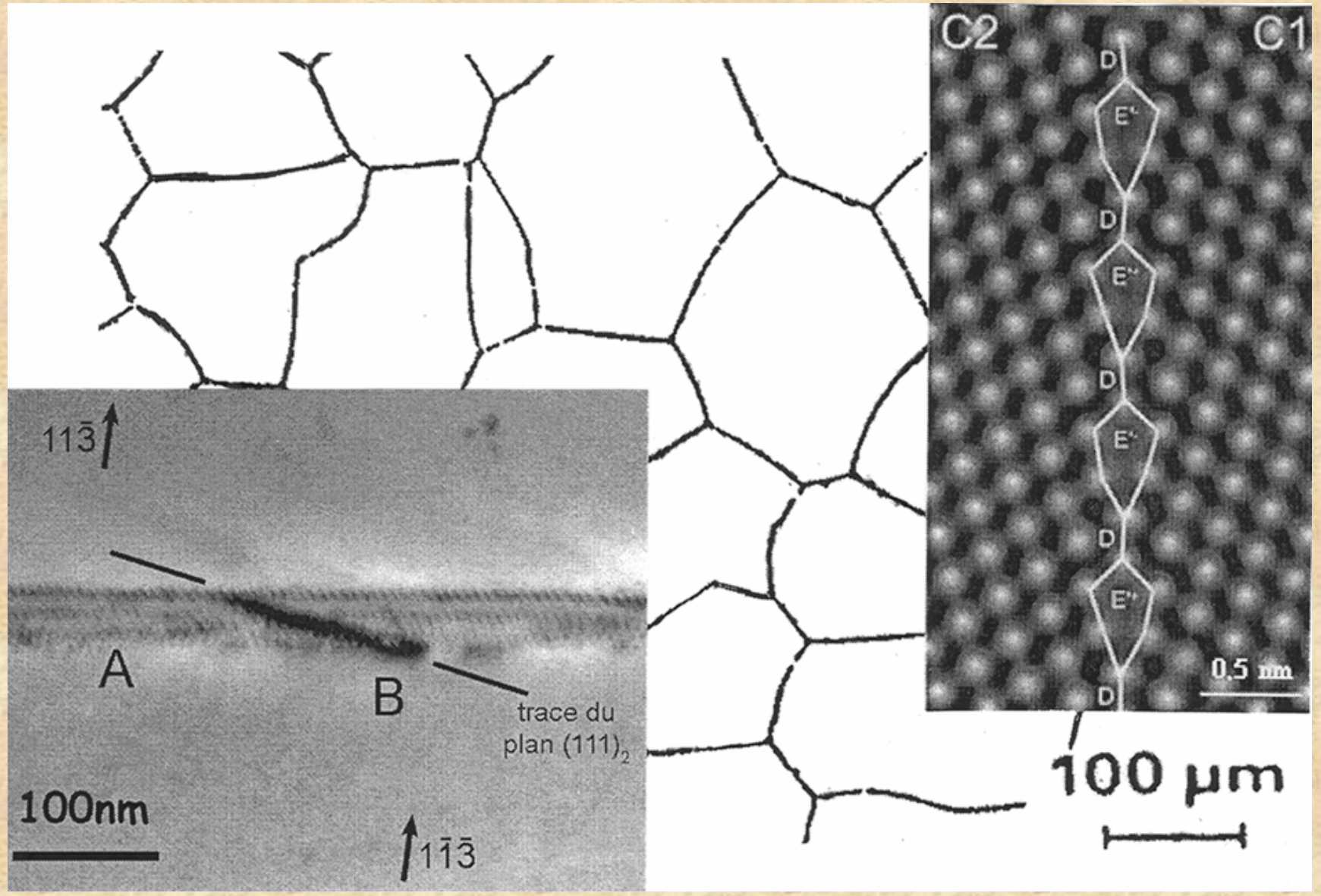
# A GRAIN BOUNDARY at DIFFERENT SCALES



# « IDEAL » GRAIN BOUNDARY

## GB equilibrium  Structure ⇒ what ORDER ?

**I - Geometrical order: Bicrystallography**

**II - Stress Order: Intrinsic Dislocations (IGBDs)**

**III - Atomic order: Structural Units (Sus)**

**IV - Correlation between intrinsic dislocations and structural units**

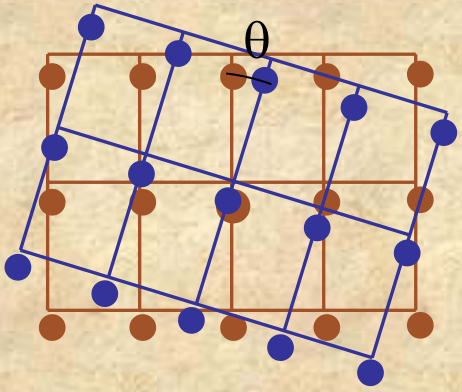
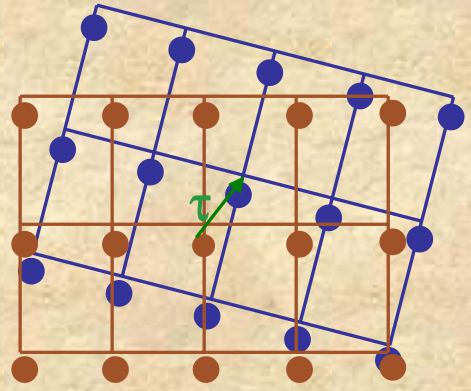
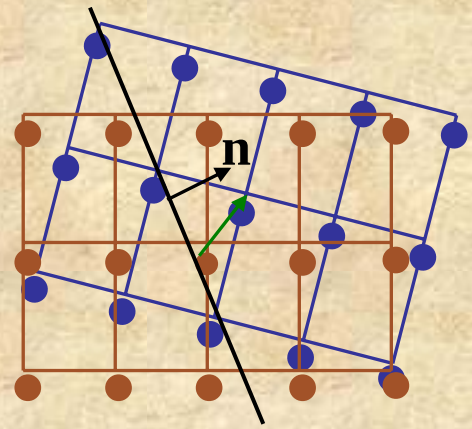
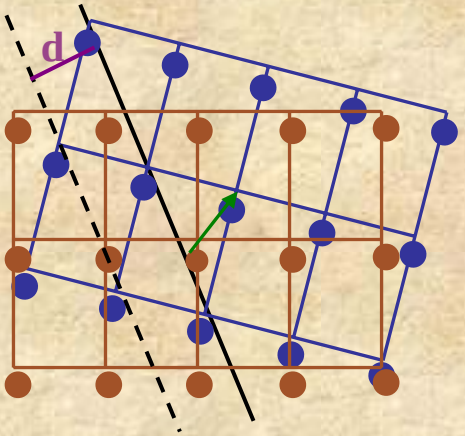
# « REAL  » GRAIN BOUNDARY

## Out of equilibrium

**V - Structural defects of grain boudaries**

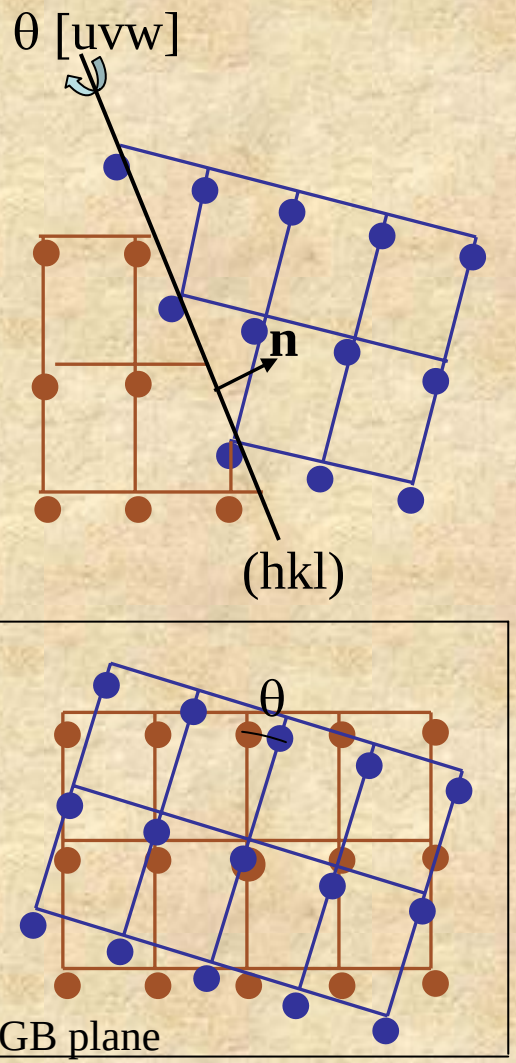
# I ) GEOMETRICAL ORDER: BICRYSTALLOGRAPHY

# GEOMETRICAL PARAMETERS OF A GRAIN BOUNDARY

| | **Macroscopic** | **Microscopic** |
|---|---|---|
| **Interface operation** *(bicrystal)* |  |  |
| **GB plane** |  |  |
| | **3** parameters for the rotation : θ **<uvw>**<br>+<br>**2** parameters for the plane orientation **n** | **3** parameters for the rigid translation τ<br>+<br>**1** parameter for the plane position **d** |

# Different types of GBs

| n, [u v w ] | GB type |
|---|---|
| n ⊥ [uvw] | Tilt GB |
| n // [uvw] | Twist GB |
| n inclined / [uvw] | Mixte GB |
| $(hkl)_1 = (hkl)_2$ | Symmetrical GB |
| $(hkl)_1 \neq (hkl)_2$ | Asymmetrical GB |



# NOTION OF COINCIDENCE

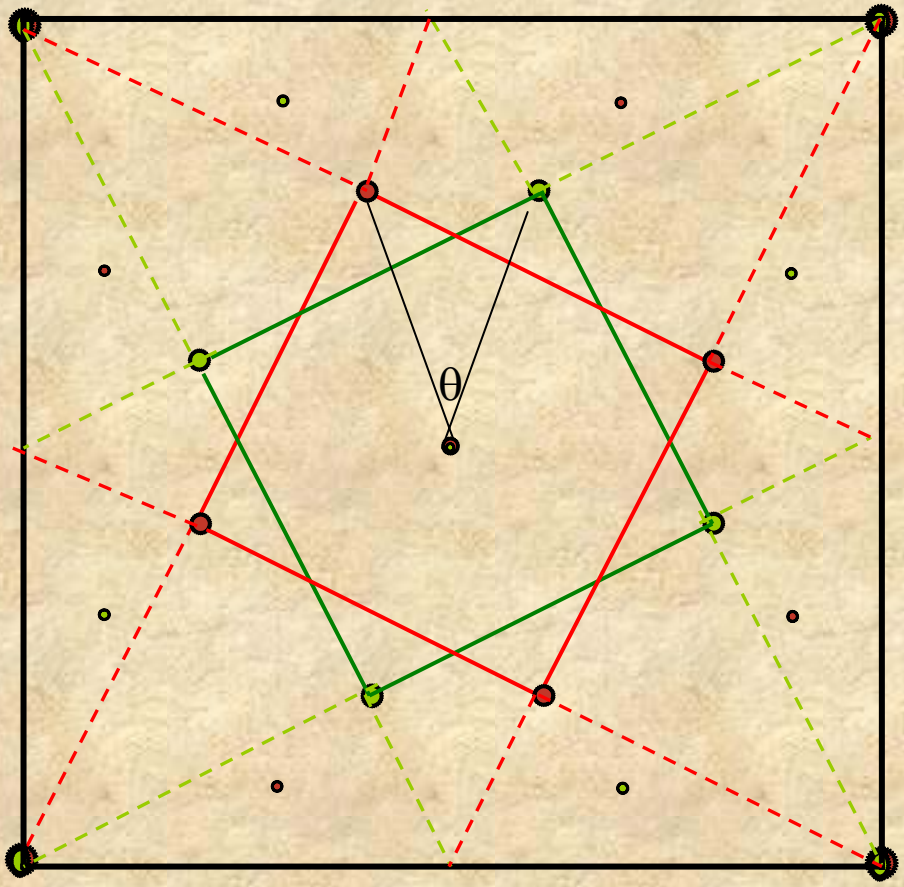
CSL

$$\Sigma = \frac{V_{CSL}}{V_{\text{primitive cell of crystal}}} = \frac{1}{\rho \text{ (density of common nodes)}}$$

For cubic symmetry

$\Sigma = 5$

$36.9^\circ$ <100>

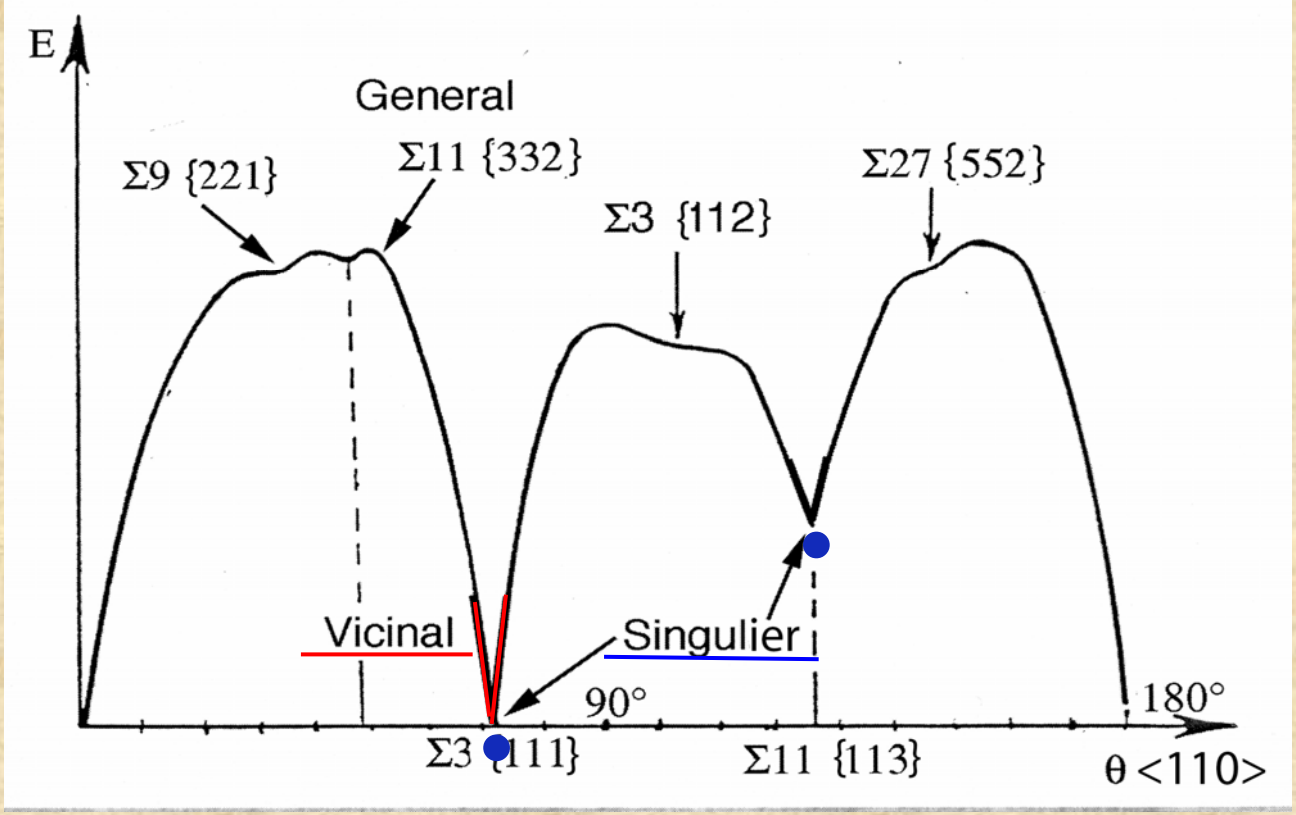



**CSL = $T_1 \cap T_2$**

*$T_1$ et $T_2$ are the translation lattices of the two crystals*

# GB ENERGY

No correlation between E et Σ




**Classification of GBs based on their energy: Singular - Vicinal - Générall**

# TRANSLATION LATTICE OF GRAIN BOUNDARY

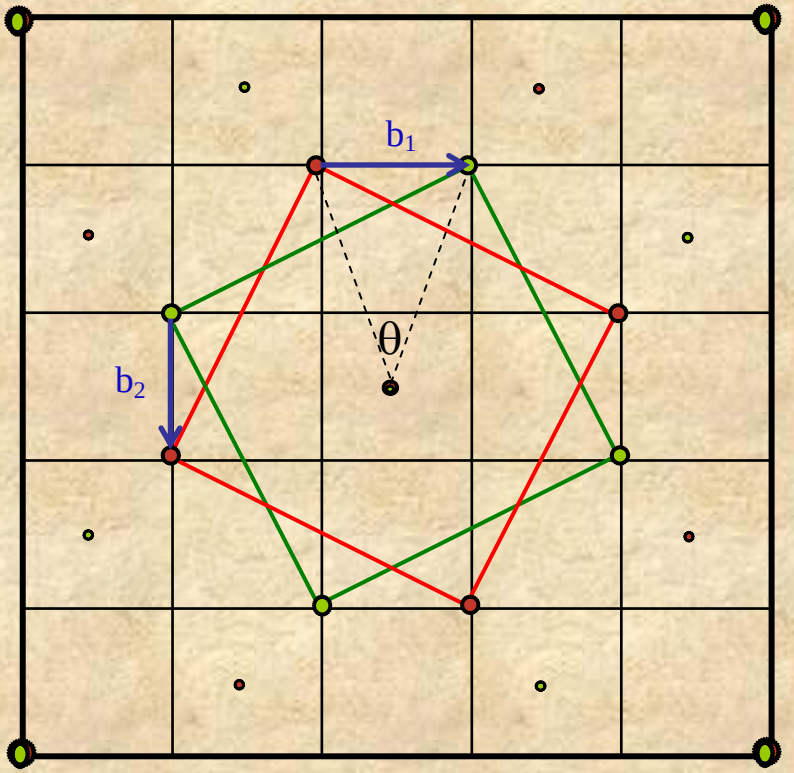
DSC

Defines the Burgers vectors of perfect GB dislocations

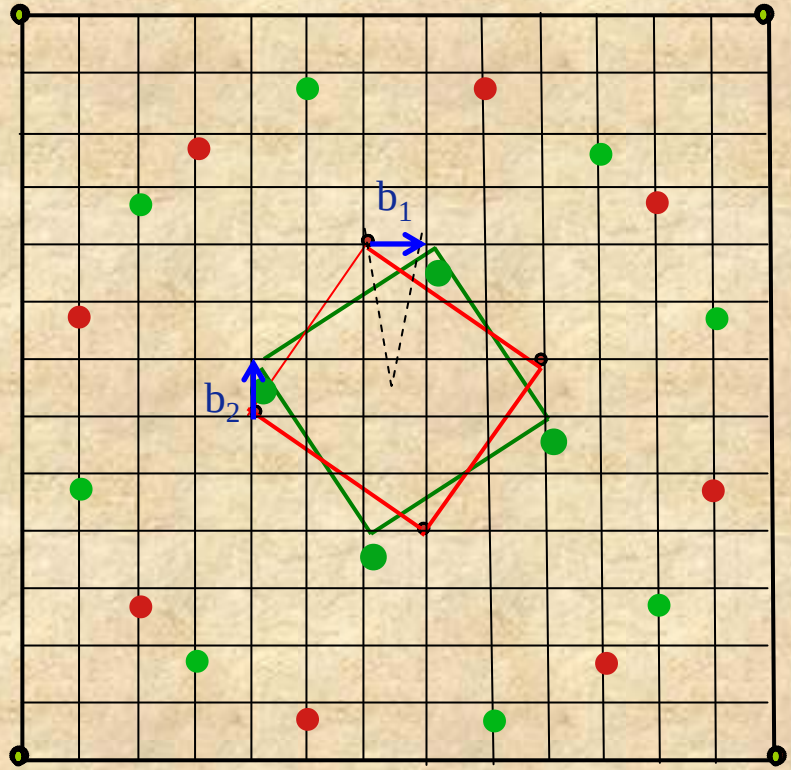
$$DSC = T_1 \cup T_2$$

$$V_{DSC} = \frac{1}{V_{CSL}}$$

If $\Sigma \rightarrow \infty \Rightarrow$ $\mathbf{b}_{DSC}$




Σ 5




Σ 13

# 0 LATTICE

Locus of invariant points in the transformation : crystal 1 $\Rightarrow$ crystal 2

## Fondamental equation

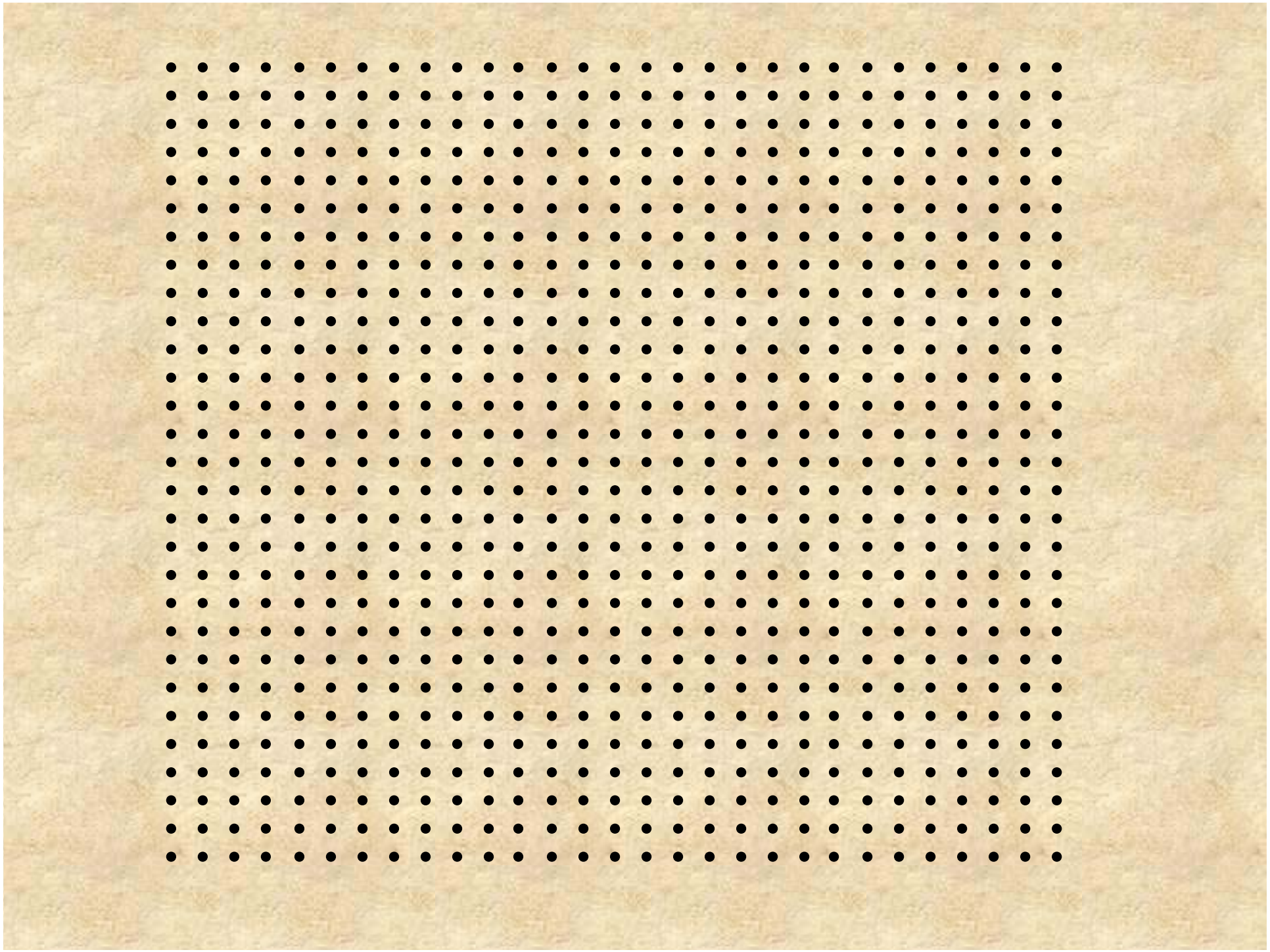
If $\tau = 0$ (Bollmann)

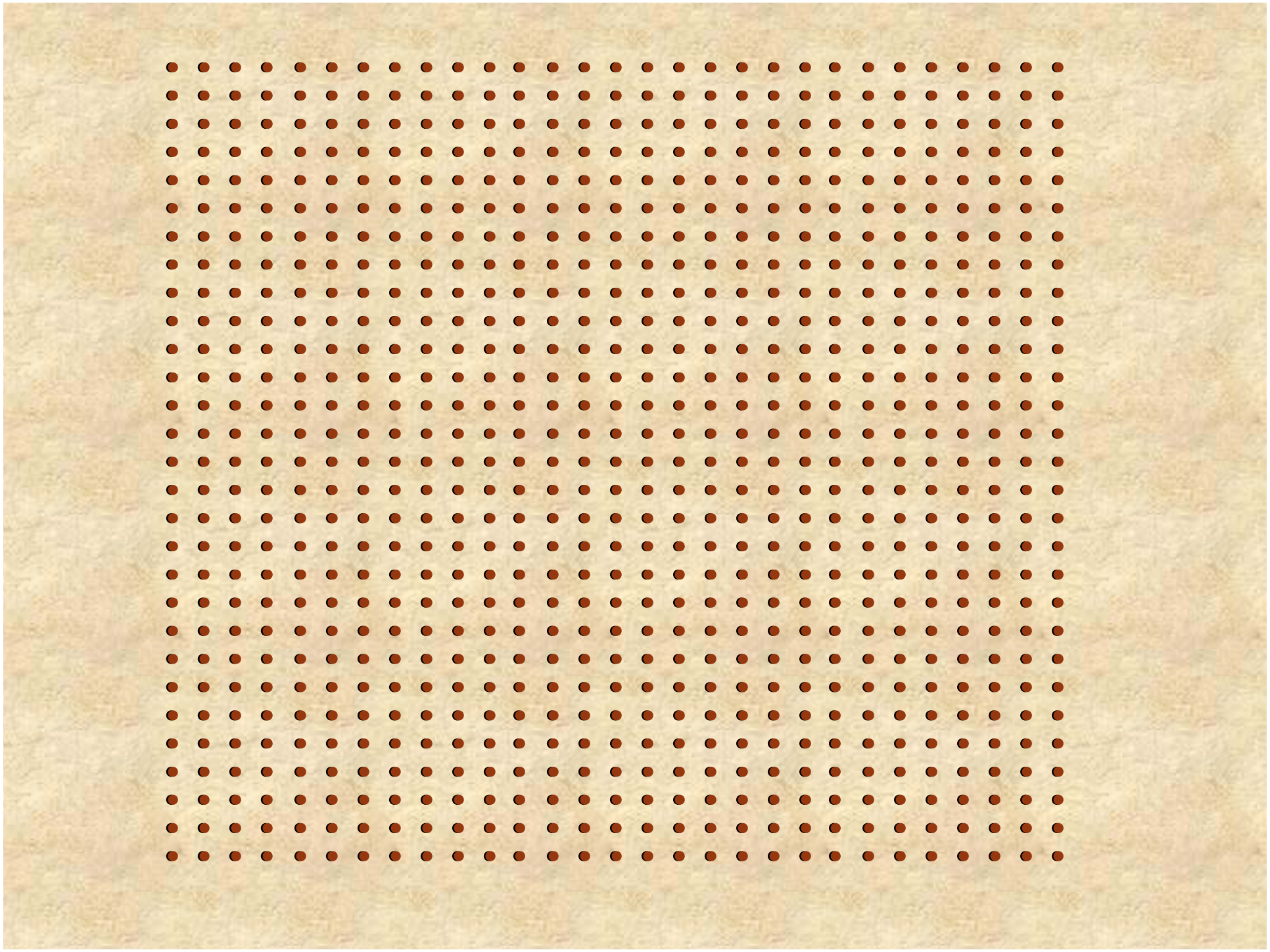
$\mathbf{x}_0 = \mathbf{R}\,\mathbf{x}_0 + \mathbf{B}_m$ $\quad$ $\mathbf{B}_m$ = translation vector in crystal

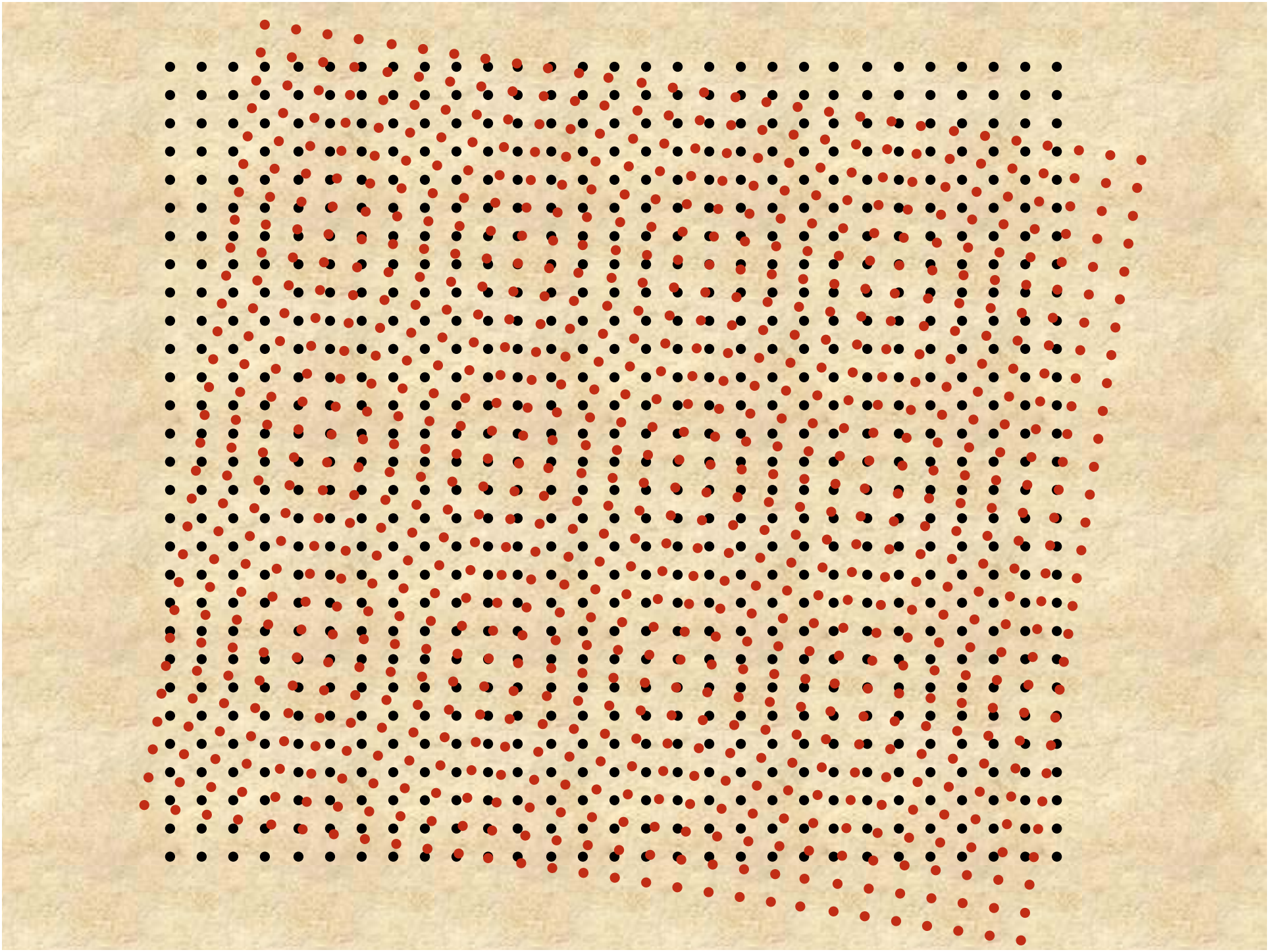
$(\mathbf{I} - \mathbf{R}^{-1})\,\mathbf{x}_0 = \mathbf{B}_m = \Sigma\,\mathbf{b}_m$ $\quad$ $\mathbf{b}_m$ = Burgers vector for crystal

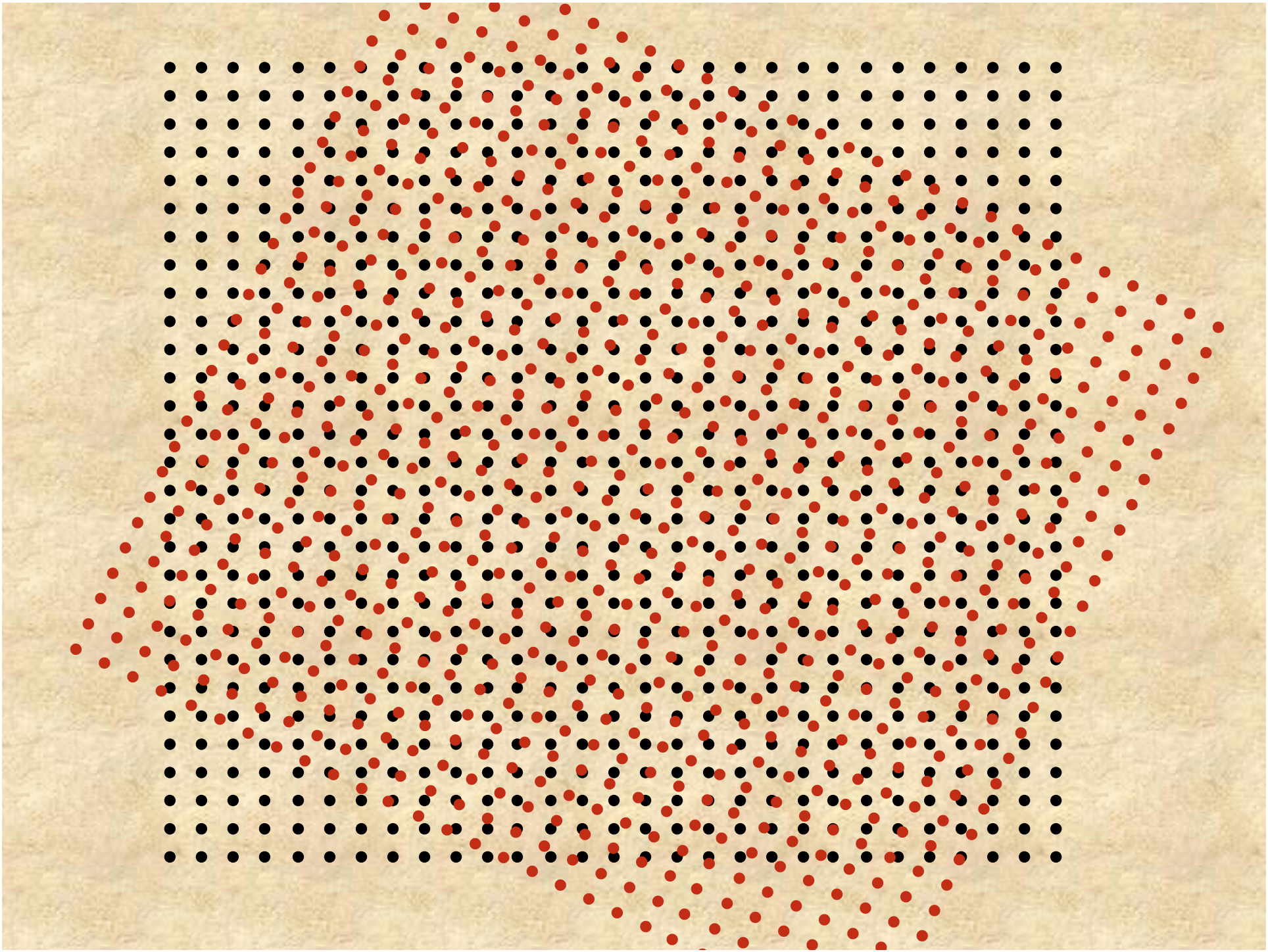
## Properties

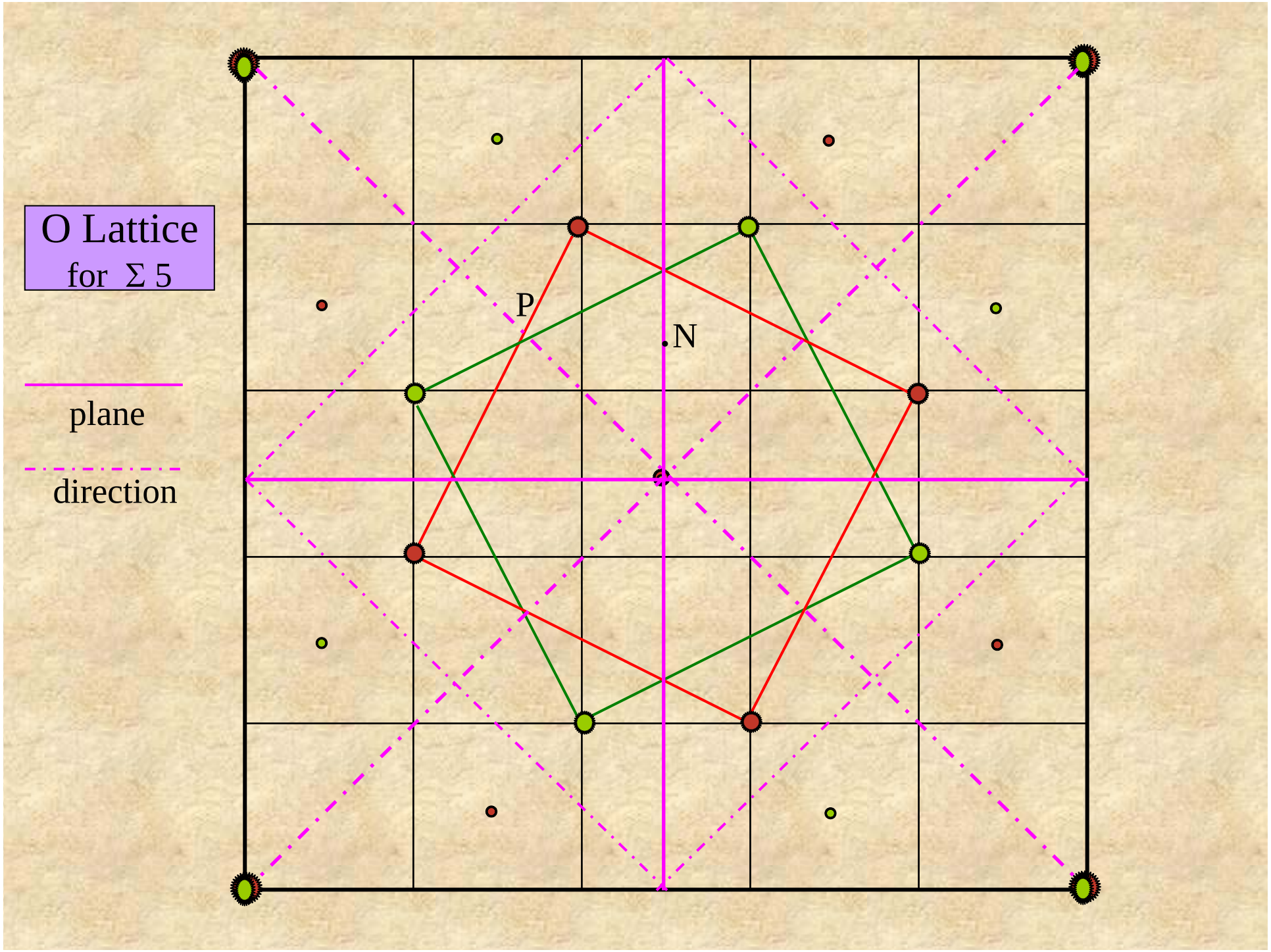
- Continuous function of the misorientation $\theta$
- Any 0 point is an origine for the rotation










O Lattice
for Σ 5
plane
direction
P
N

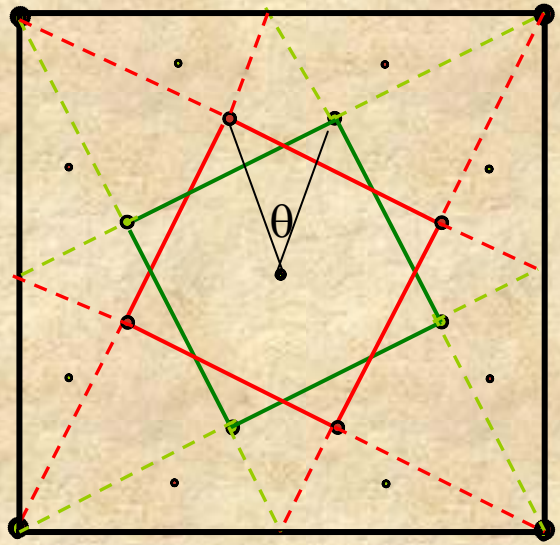
## O2 LATTICE

Real GB : $\theta = \theta_{coincident} + \Delta\theta$

$\mathbf{x}_2 = \mathbf{R}' \mathbf{x}_1$ $\quad$ $\mathbf{x}_2 = \mathbf{R}\, \mathbf{x}_1$

$\mathbf{R}'\mathbf{R}^{-1} = \mathbf{D}$

**D** : Deviation matrix




The coincidence lattice is a second invariant

**Fondamental equation**

$$(\mathbf{I} - \mathbf{D}^{-1})\, \mathbf{x}_{02} = \Sigma\, \mathbf{b}_{DSC}$$

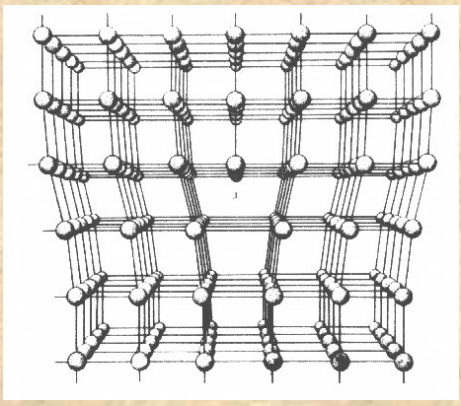
Locus of the invariant points in the D transformation

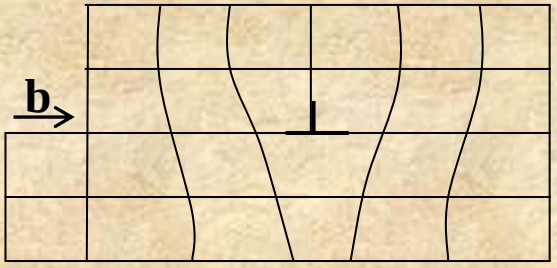
# II ) STRESS ORDER :

# INTRINSIC DISLOCATIONS

# LINEAR and PLANAR DEFECTS

## Dislocation

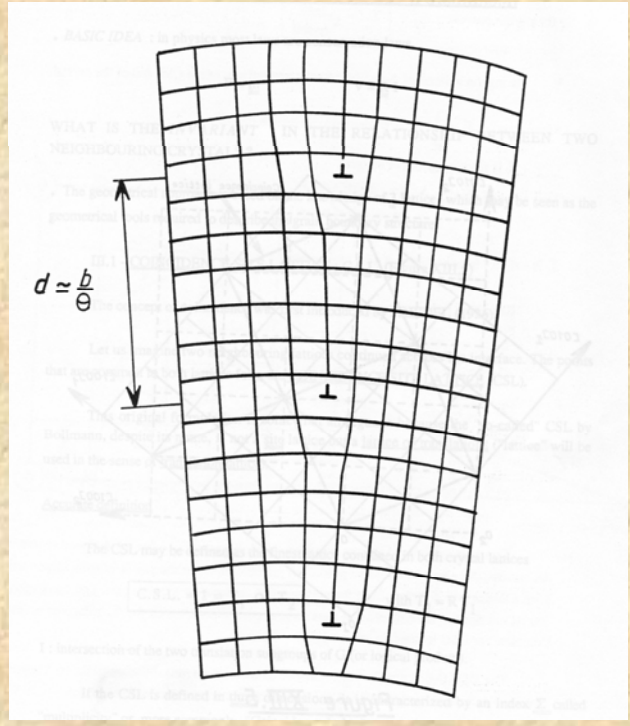






Elemental plastic deformation
**b** : translation lattice vector

## Grain Boundary



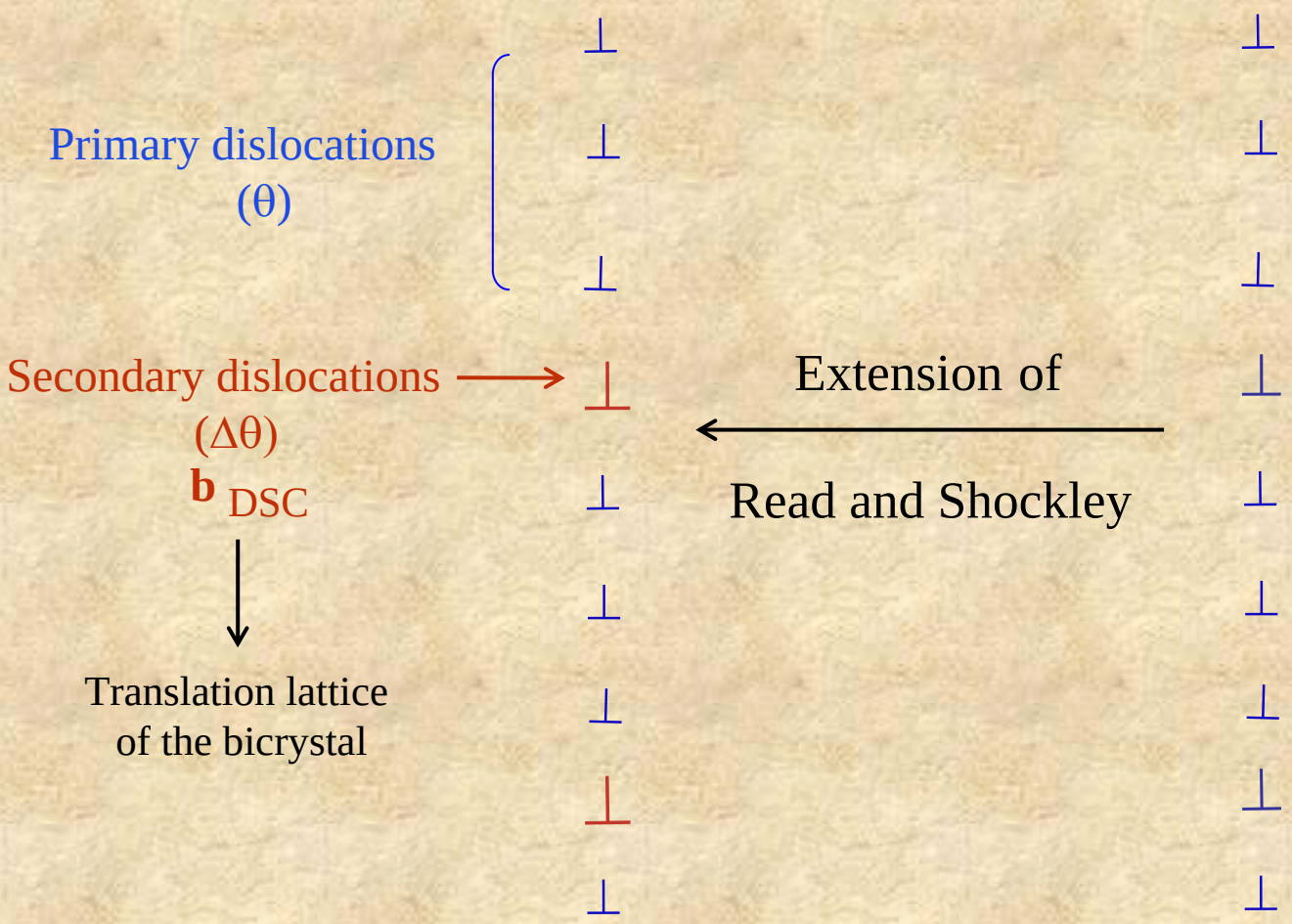

***Read and Shockley model***

$E_J = n\,E$ $\Rightarrow$ $E_J = E_0\theta\,(A - \ln\theta)$

dislocation

The stress fields of neighbouringdislocations annihilate

# BOLLMAN's MODEL for any GRAIN BOUNDARY




**Any large angle GB**

**Low angle GB**

# INTRINSIC DISLOCATIONS (Bollmann)

## Discretization of the deformation

For energetic reason, the GB tries to maintain a maximum number of common sites:
- of the single crystal ⇒ Points 0
- of the coincidence lattice ⇒ Points 02

The stresses are localized between the regions of good fit (good material)

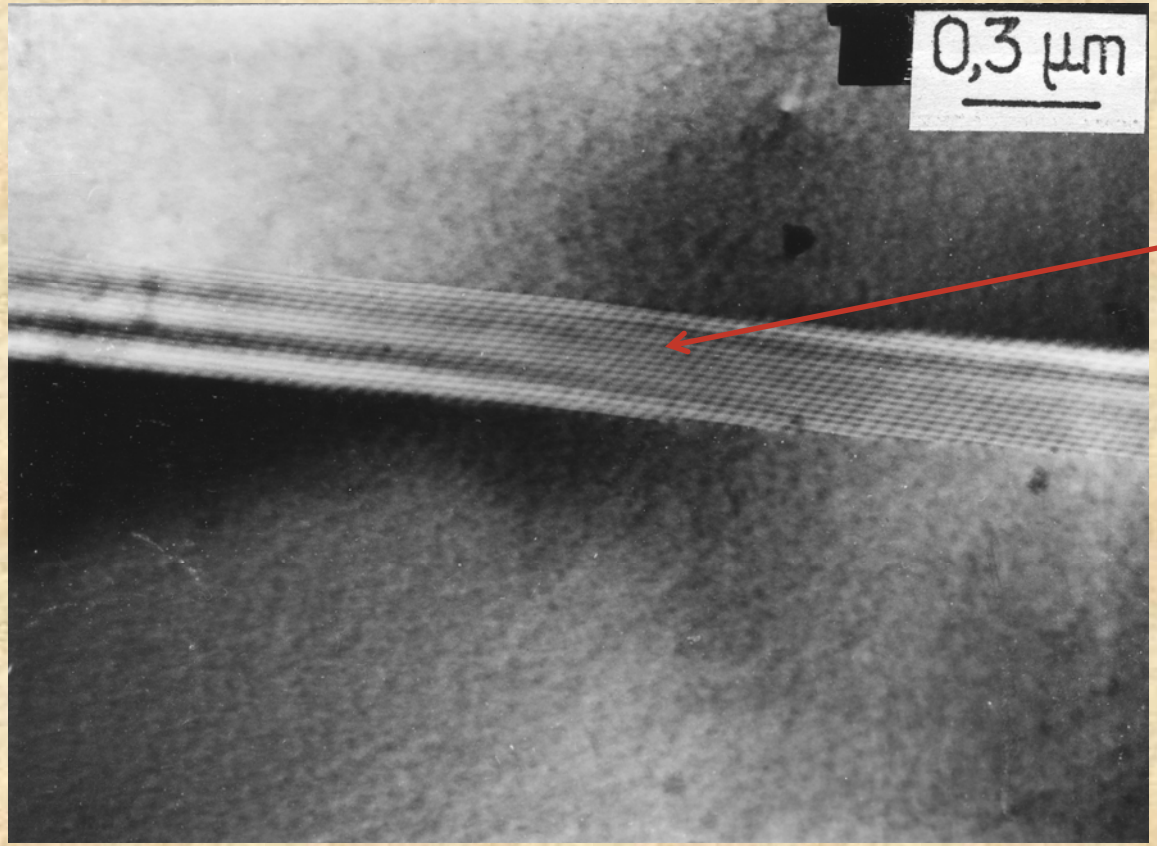
⇓

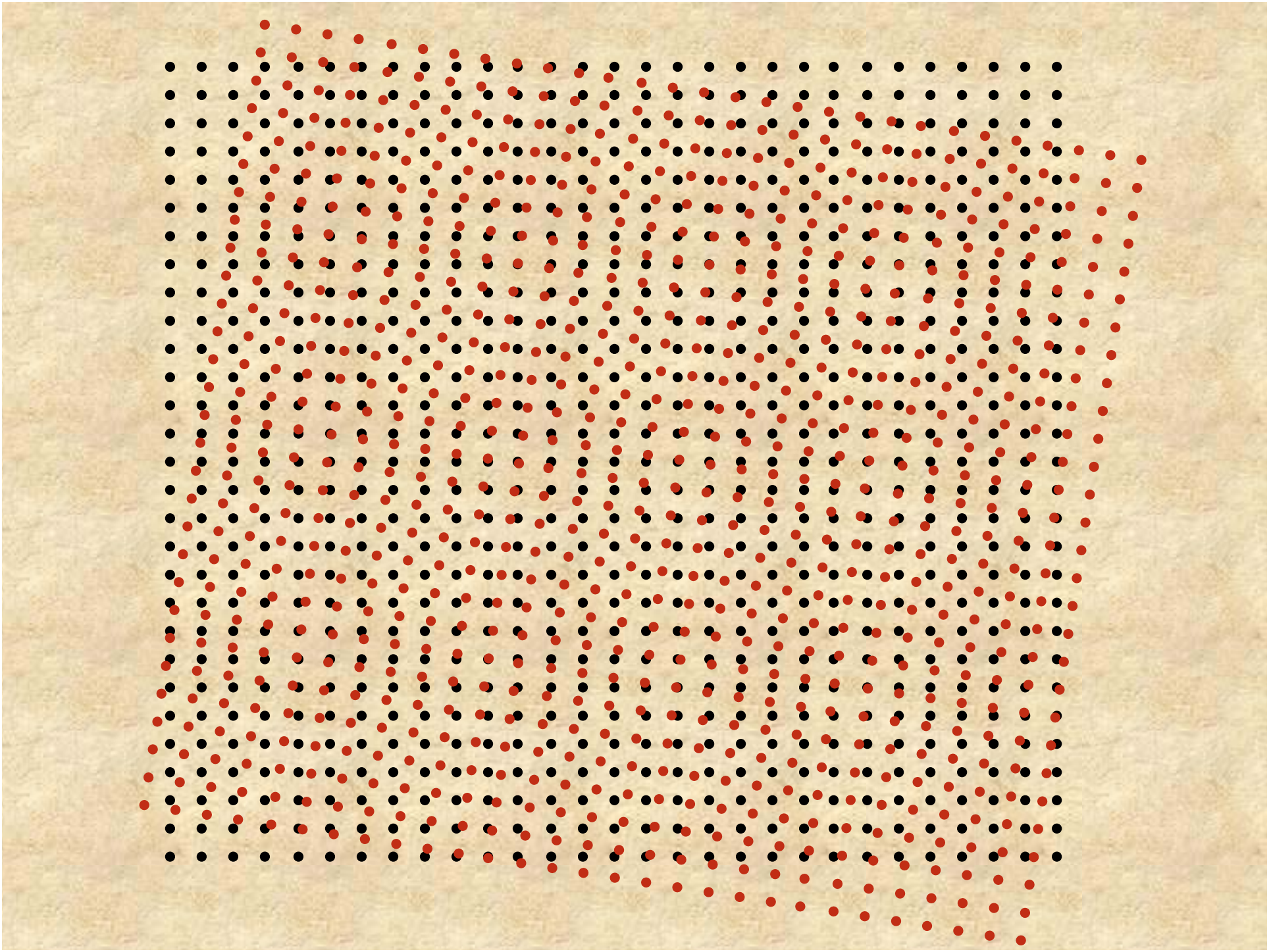
Intrinsic dislocations (bad material)

| 2 Invariants | Deviation | Good fit | Bad fit | What GB ? |
|---|---|---|---|---|
| Crystal | θ | 0 lattice<br>Common points of the two crystal lattices | Primary Dislocations<br>$\mathbf{b} = \mathbf{b}_m$ | Low angle GBs<br>Coincident GBs |
| CSL | Δθ | 02 lattice<br>**Common points of the two DSC lattices** | Secondary Dislocations<br>$\mathbf{b} = \mathbf{b}_{DSC}$ | Any GB |

# Primary intrinsic dislocations in a tilt GB

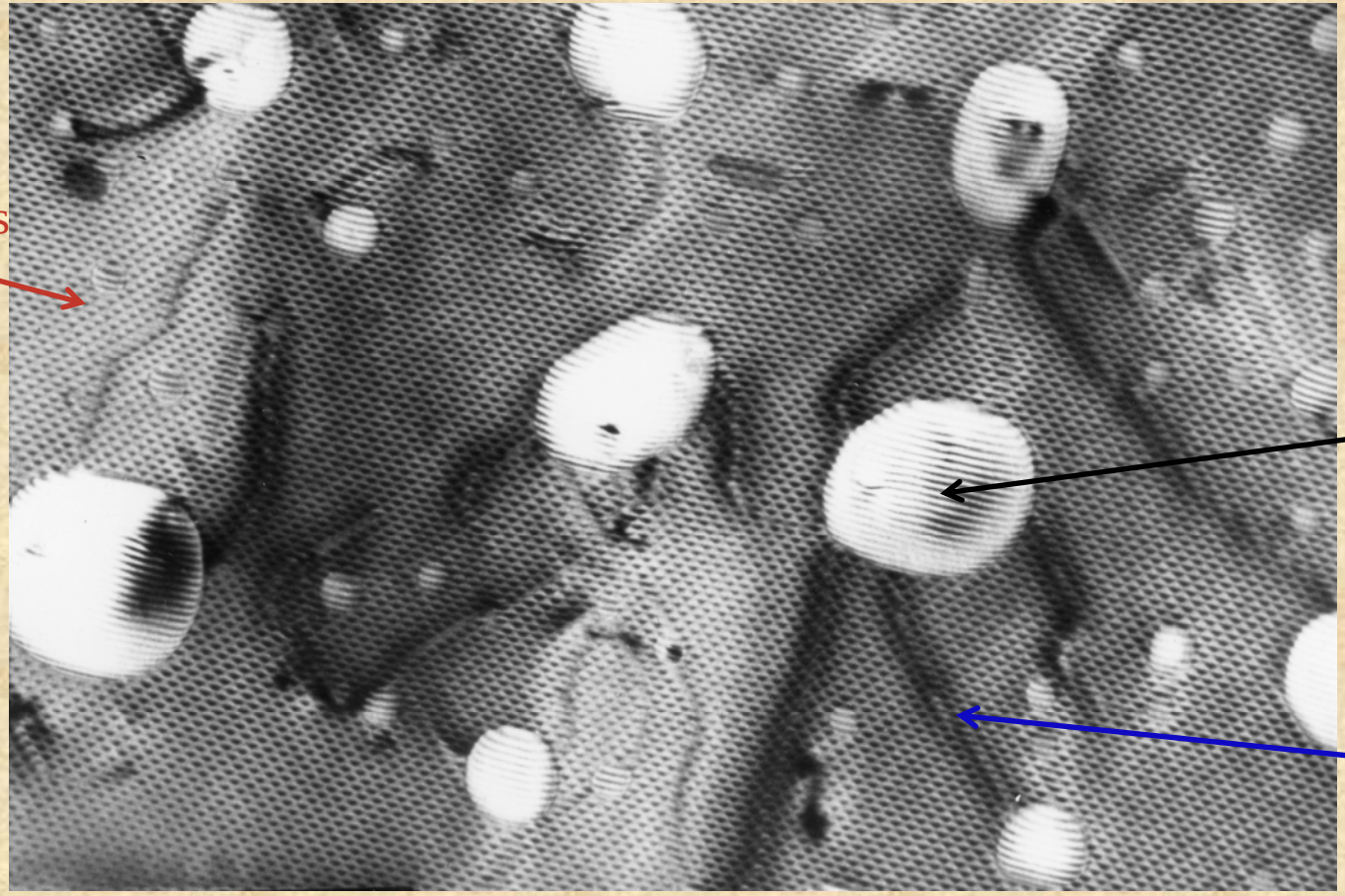
**Material:** Fe - % Mo - 100ppm C **GB:** $\theta < 2^{\circ}$





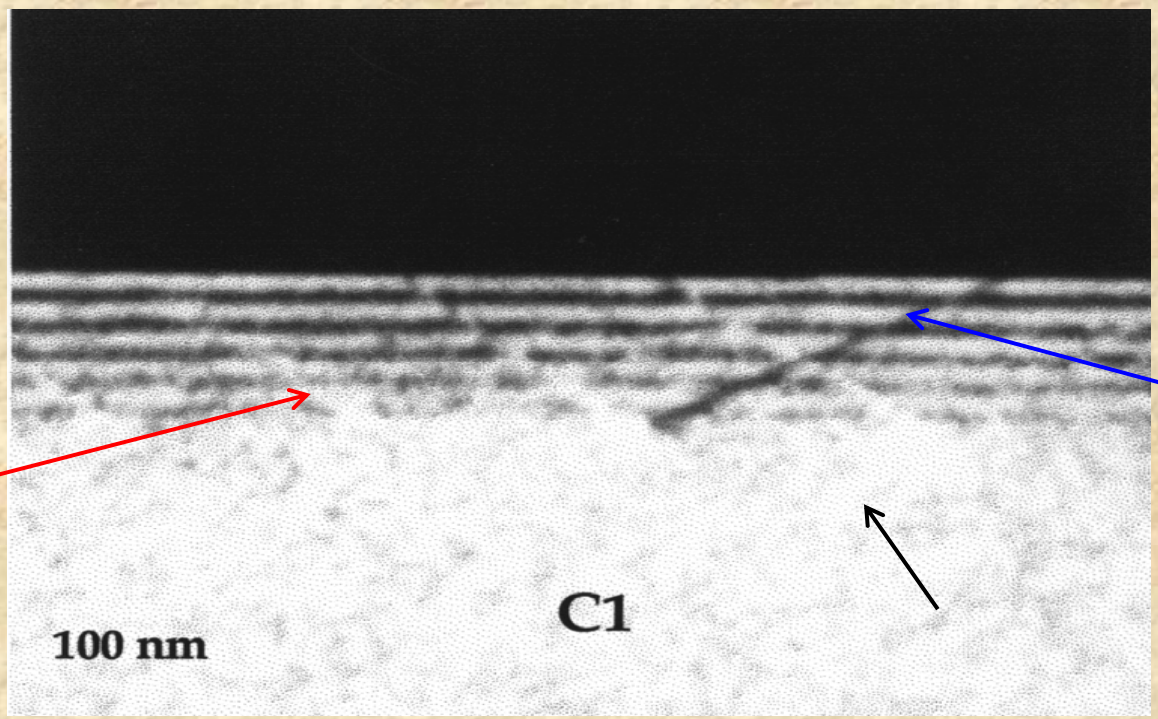
**Example of primary intrinsic dislocations (IGBDs) in a twist GB**

**$\theta \approx 3^\circ$ in gold**



# Example of secondary intrinsic dislocations (IGBDs)

$\Sigma = 3$ {111} GB in nickel - $\Delta\theta = 0.09^{\circ}$

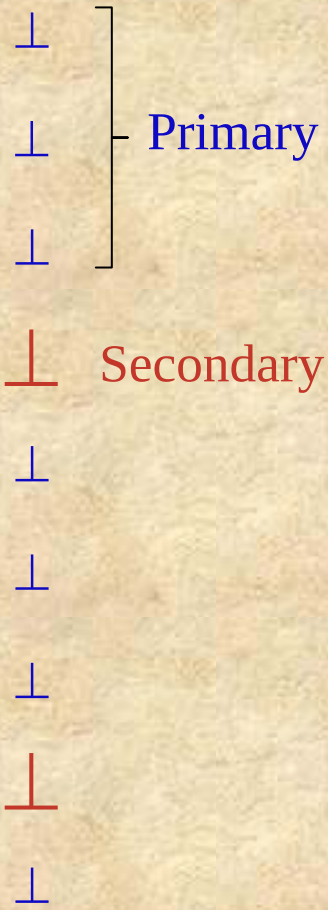



Secondary IGBD

EGBD

# INTRINSIC G.B. DISLOCATION MODEL SHORTCOMINGS

STRESS ORDER




BUT

Geometrical models rest on macroscopic parameters only

Infinity of descriptions due to symmetry ⇒ different B density

For one and only objet ??

⇓

Discretization of B depends on Relaxation processes (rigid, atomic)

No ENERGY prediction

**then**

ATOMIC ORDER

# III ) ATOMIC  ORDER: STRUCTURAL UNIT MODEL

# ATOMIC ORDER : STRUCTURAL UNIT MODEL

- Geometrical consideration (hard spheres)
- Simulations
- HRTEM

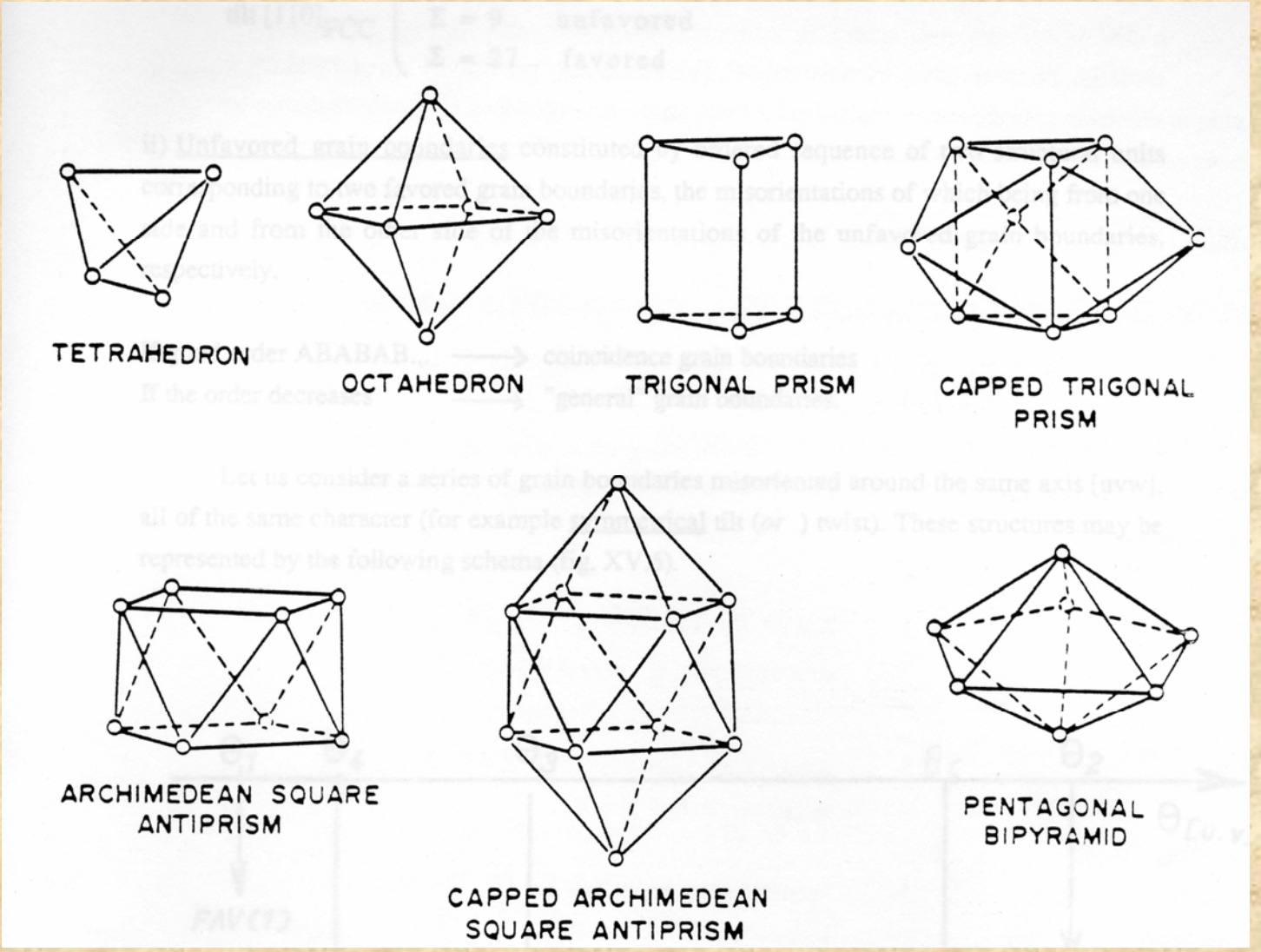
} ENERGY, STRUCTURE

**Energy localisation** ⇒ GB width ≈ 0.5 nm

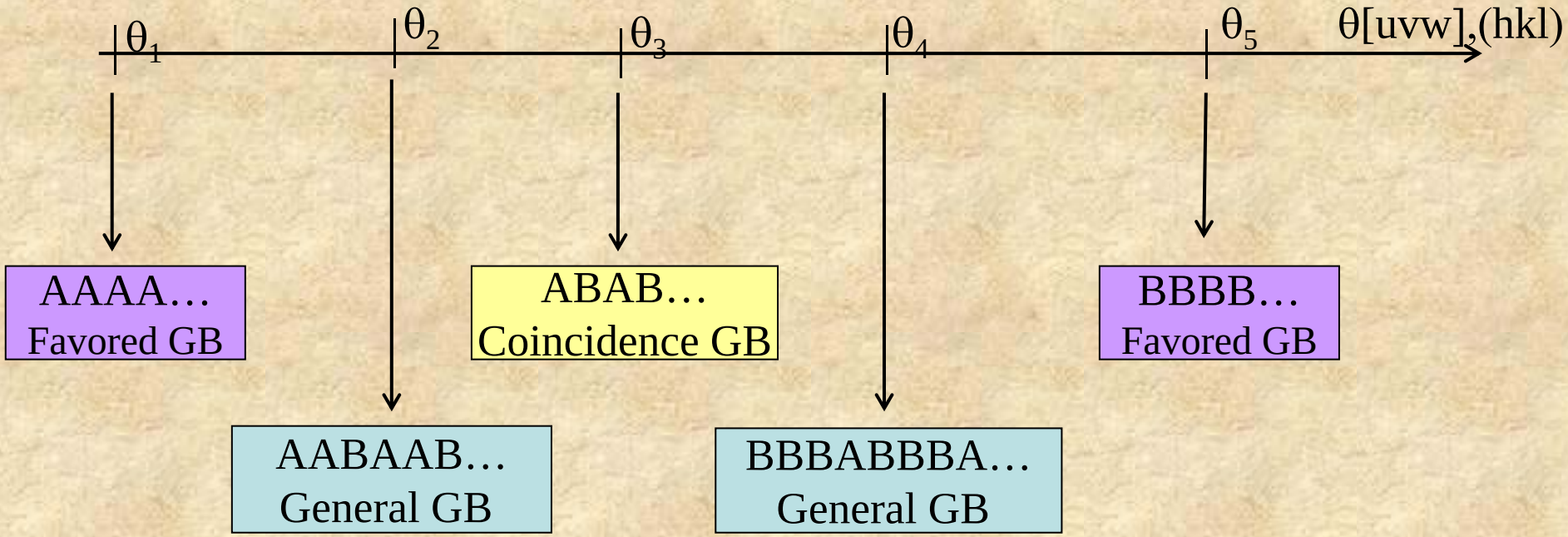
**Fine GB structure** ⇒ Any GB is constituted by polyedral units of atoms
Structural Unit (similarity with elemental cells of crystal)

**Energy by sites** ⇒ Prevision of the interstitial and substitutional sites
⇓
SEGREGATION

# DIFFERENT STRUCTURAL UNITS FOUND IN GRAIN BOUNDARIES



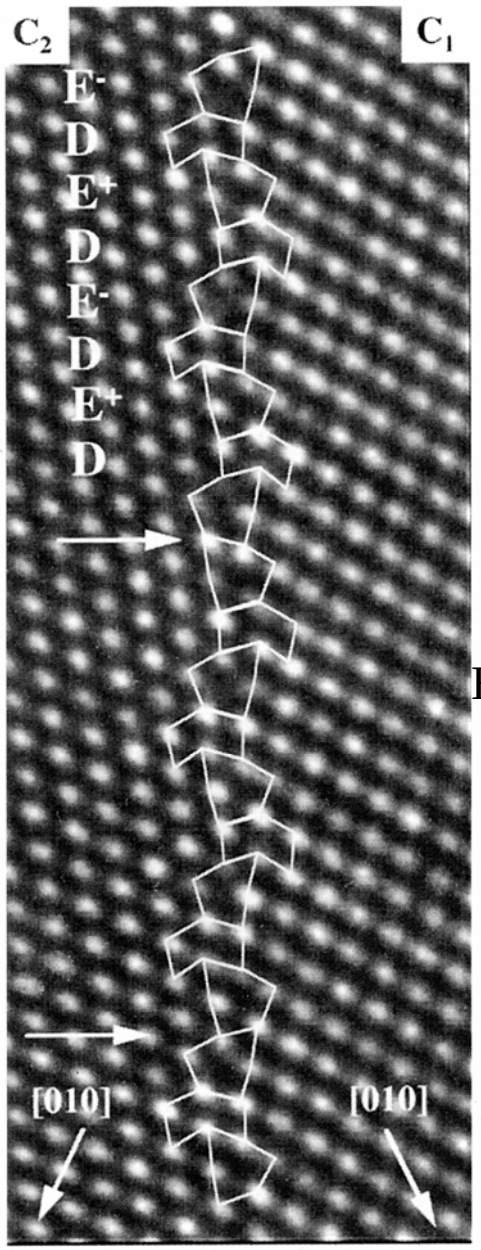
# ATOMIC ORDER : STRUCTURAL UNIT MODEL



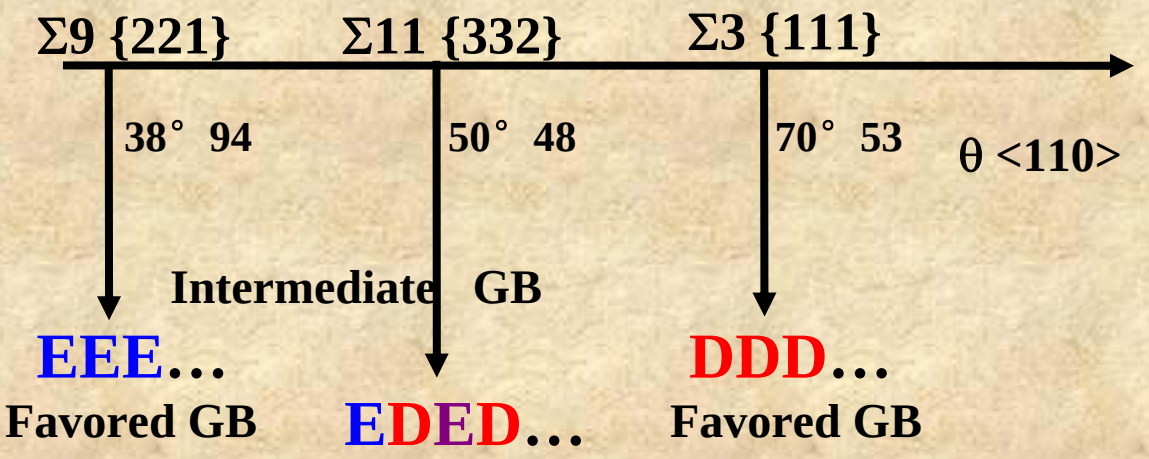

**GB period** : $\mathbf{p} = m\,\mathbf{u}_A + n\,\mathbf{u}_B$

simple principle BUT COMPLEXITY →
- Distortion of the SUs
- Multiplicity of descriptions
- Hierarchy of descriptions

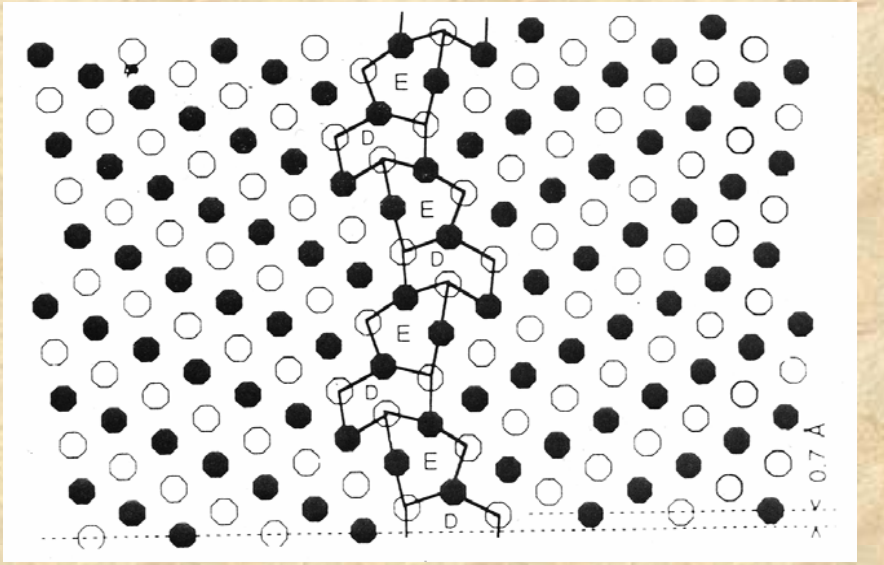
## Description in terms of Structural Units (SU)



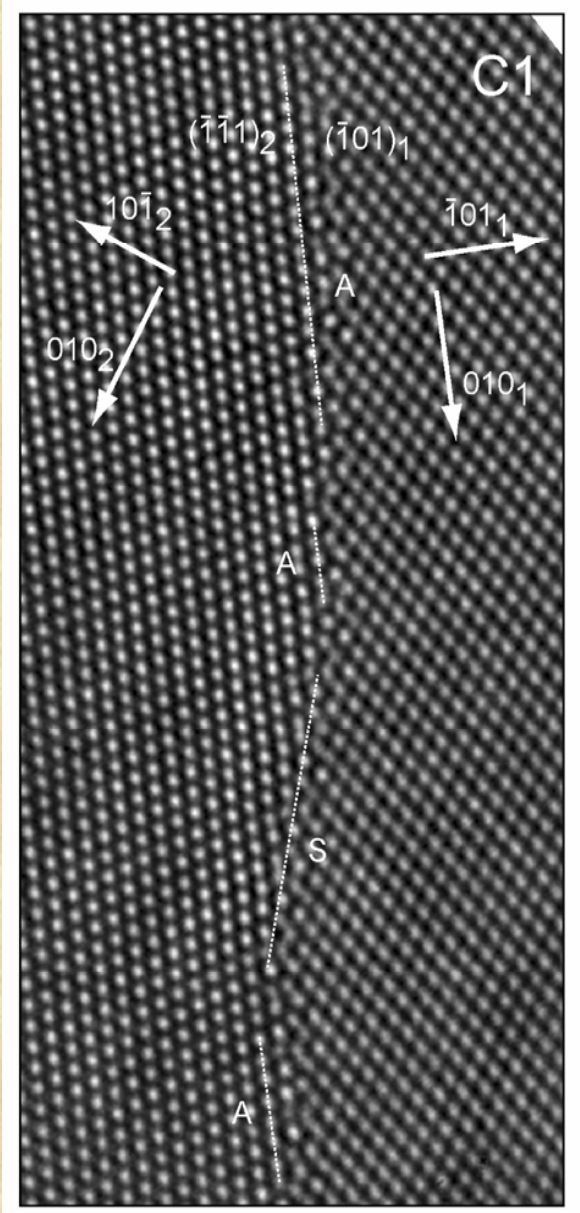

HRTEM image

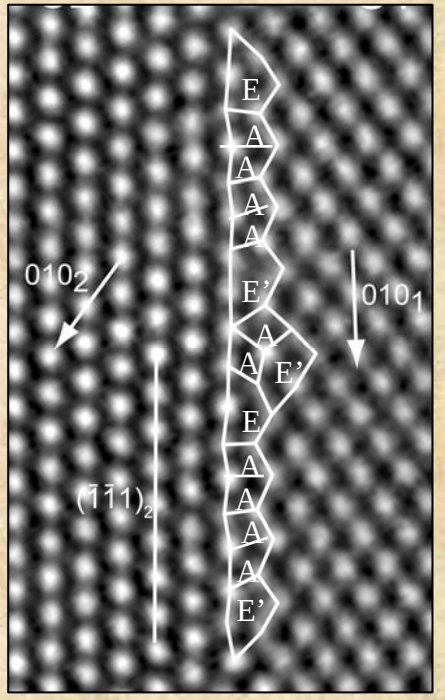


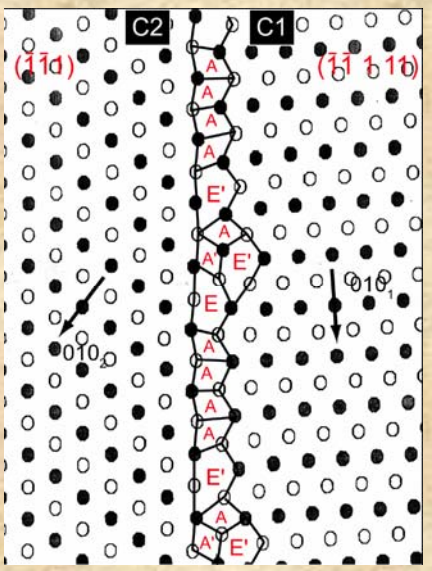

Simulation



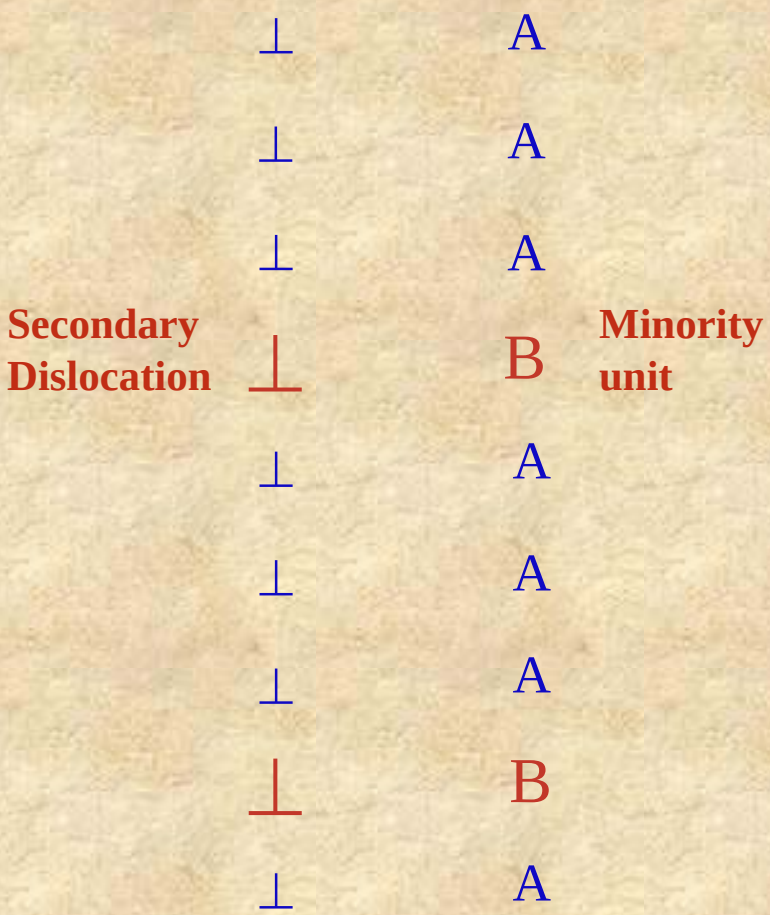
# FACETING GB near Σ 9 in COPPER



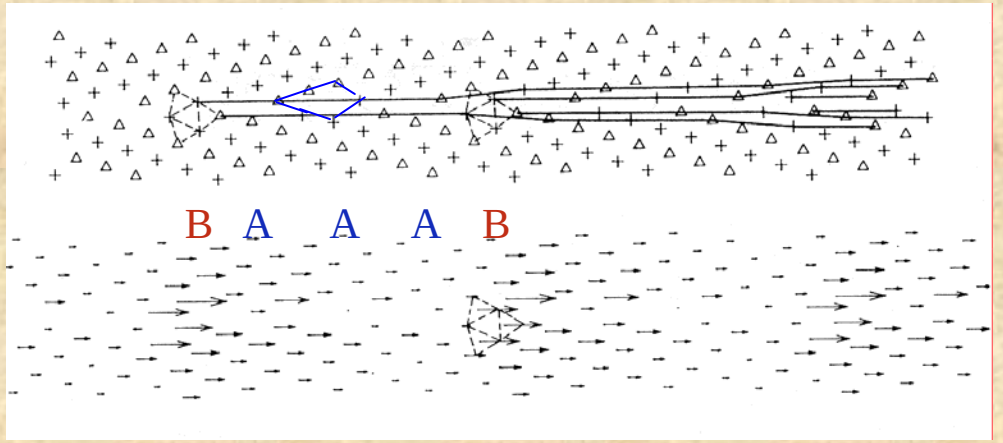



# STRUCTURAL UNITS/ INTRINSIC DISLOCATIONS




Each minority unit B is the core of a secondary dislocation with a DSC Burgers vector of the delimiting GB composed of A units.




Symmetrical GB Σ 89 {229}in aluminum

# SU /GBD MODEL USEFULNESS AND SHORTCOMINGS

## USEFULNESS

Prediction of the atomic structure of pure tilt GBs and pure twist GBs around axes with low indices: <100>, <110> and <111>

## SHORTCOMINGS

**Geometry**

- Tilt and twist GBs around axes with high indices
- Mixed GBs
- Delimiting GBs with rigid body translation

**Material**

- Low SFE materials ⇒ 3D GBs
- What limit for the SU distortion (metals) ?

## EXTENSION TO QUASICRYSTALLINE GBs

Any GB
⇓
Long range order

→ + translational symmetry ⇒ **Periodic** Structure

→ **No** translational symmetry ⇒ **Quasiperiodic** structure

# IV) GRAIN BOUNDARY DEFECTS
## EXTRINSIC DISLOCATIONS

# GRAIN BOUNDARY EXTRINSIC DISLOCATIONS

Extrinsecus = from Outside


$\mathbf{B + b_m}$ $\qquad$ $\mathbf{B + \Sigma\, b_{DSC}}$

$\Rightarrow$

Towards equilibrium

$$\frac{B + \Sigma\, b_{DSC}}{B'} = 1$$

$\mathbf{R \Rightarrow R'}$

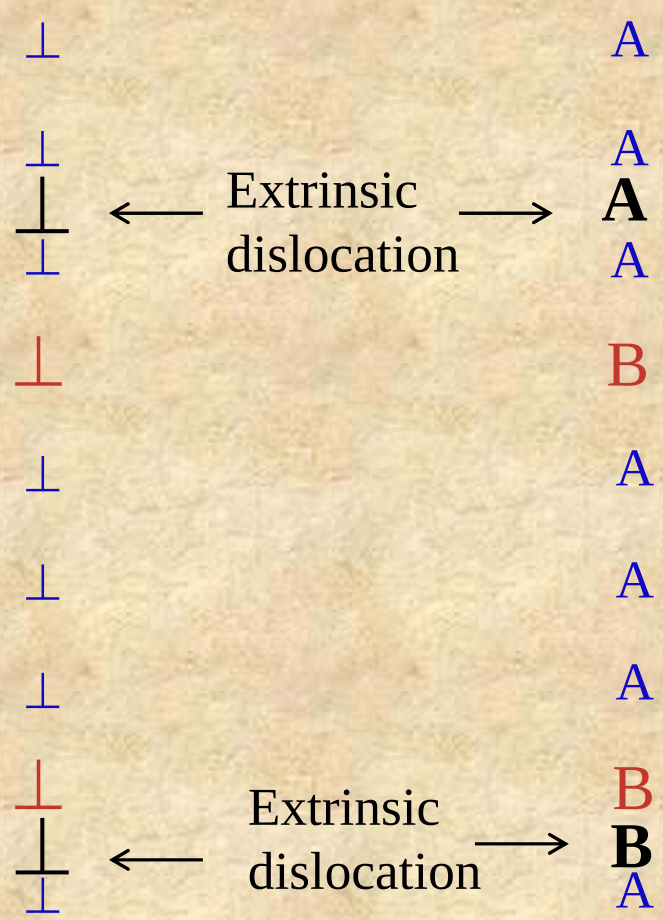
$\mathbf{(I - R'^{-1})\, p = B'}$

EXTRINSIC = NON EQUILIBRIUM $\Rightarrow$ LONG RANGE STRESSES

$\Downarrow$ **Accommodation**

INTRINSIC = EQUILIBRIUM $\Rightarrow$ SHORT RANGE STRESSES

# EXTRINSIC DISLOCATIONS/STRUCTURAL UNITS




Defect = Rupture of periodicity

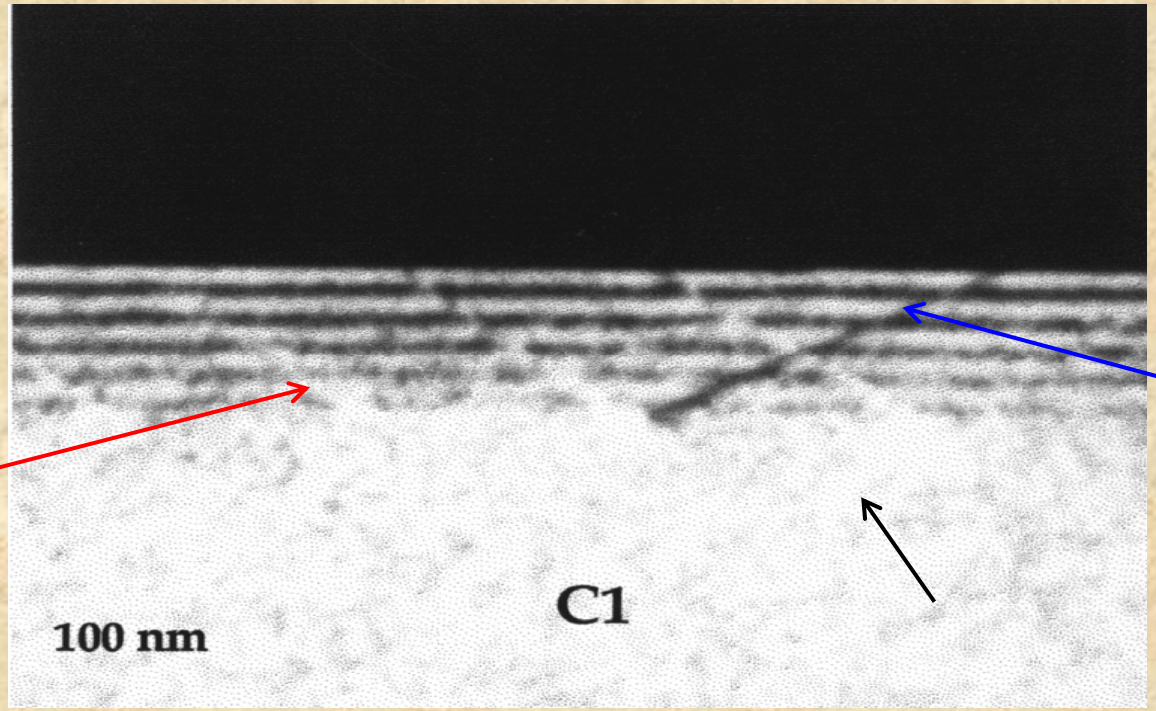
Addition or removal of one SU
≡ Extrinsic dislocation

⇓

**b** must be compatible with
the GB structure

# Example of Extrinsic Grain Boundary Dislocations (EGBDs) in a tilt GB

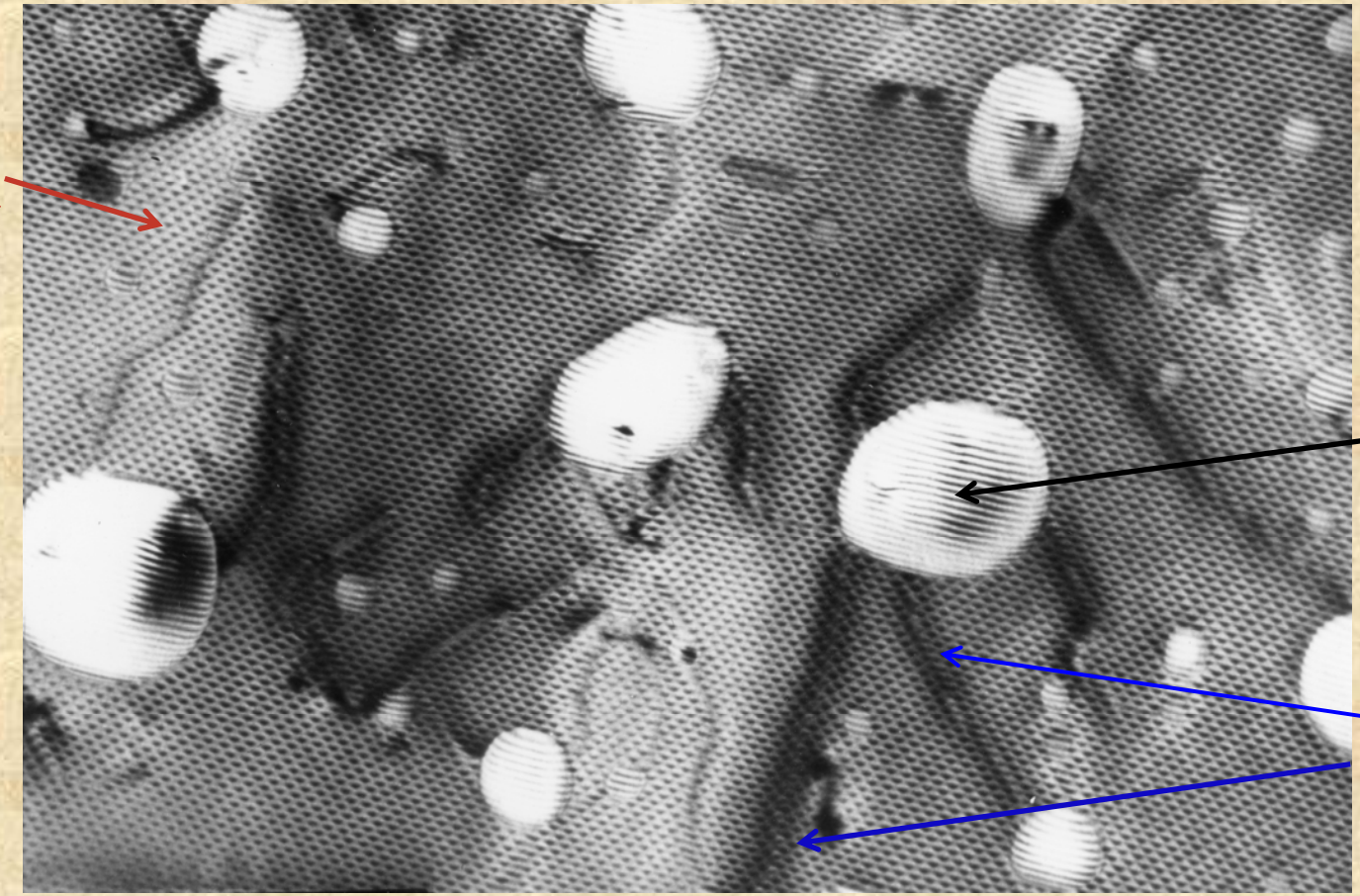
Near Σ 3 GB in copper




**Intrinsic dislocations**

**Extrinsic dislocation**

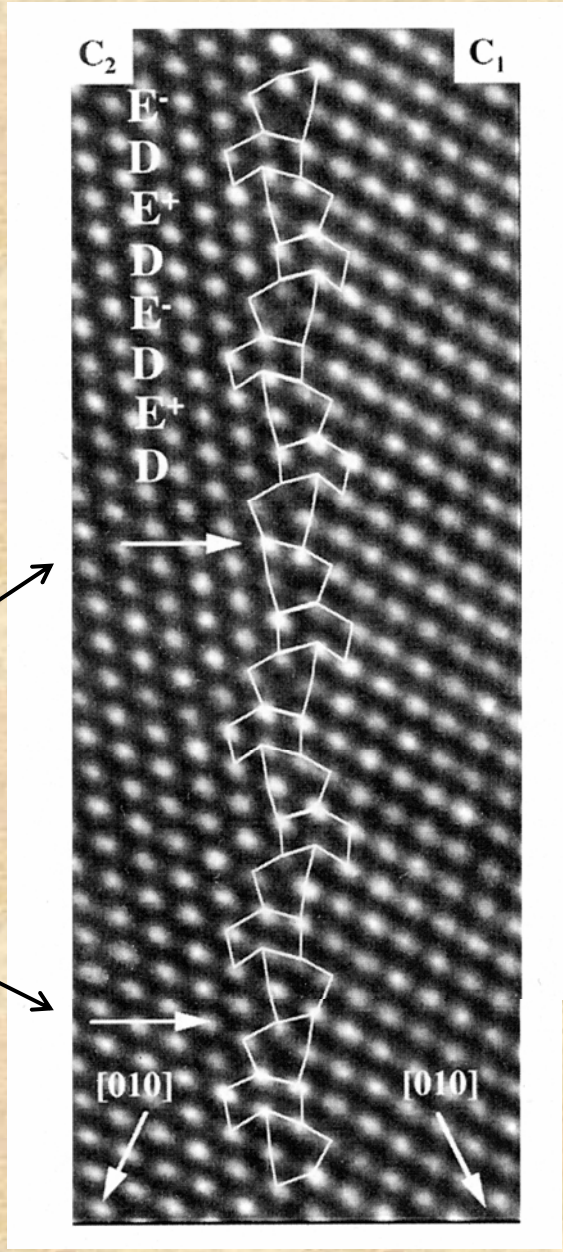
# Example of Extrinsic Grain Boundary Dislocations (EGBDs) in a twist GB




Note the strong EGBD image constrast compared to that of the IGBDs

# Example of EGBD/ SU in Σ11 {332} in nickel

The absence of a Σ3 SU corresponds to the presence of a sessile EGBD with $b_{DSC}$ = a/22 <323>



# EQUILIBRIUM / NON EQUILIBRIUM

| | | CRYSTAL | GRAIN BOUNDARY |
|---|---|---|---|
| EQUILIBRIUM | Periodic arrangement of atoms | 3D | 2D and Periodic network of intrinsic dislocations |
| DEFECTS | Point | Vacancies<br>Substitutional<br>Interstitial | Vacancies<br>**Segregated atoms *** |
| | **Linear** | Dislocation | **Extrinsic dislocation** |
| | Planar | Stacking faults<br>Grain boundaries | Facets |
| | Volume | Precipitates | **Precipitates *** |

*** Second lecture**