

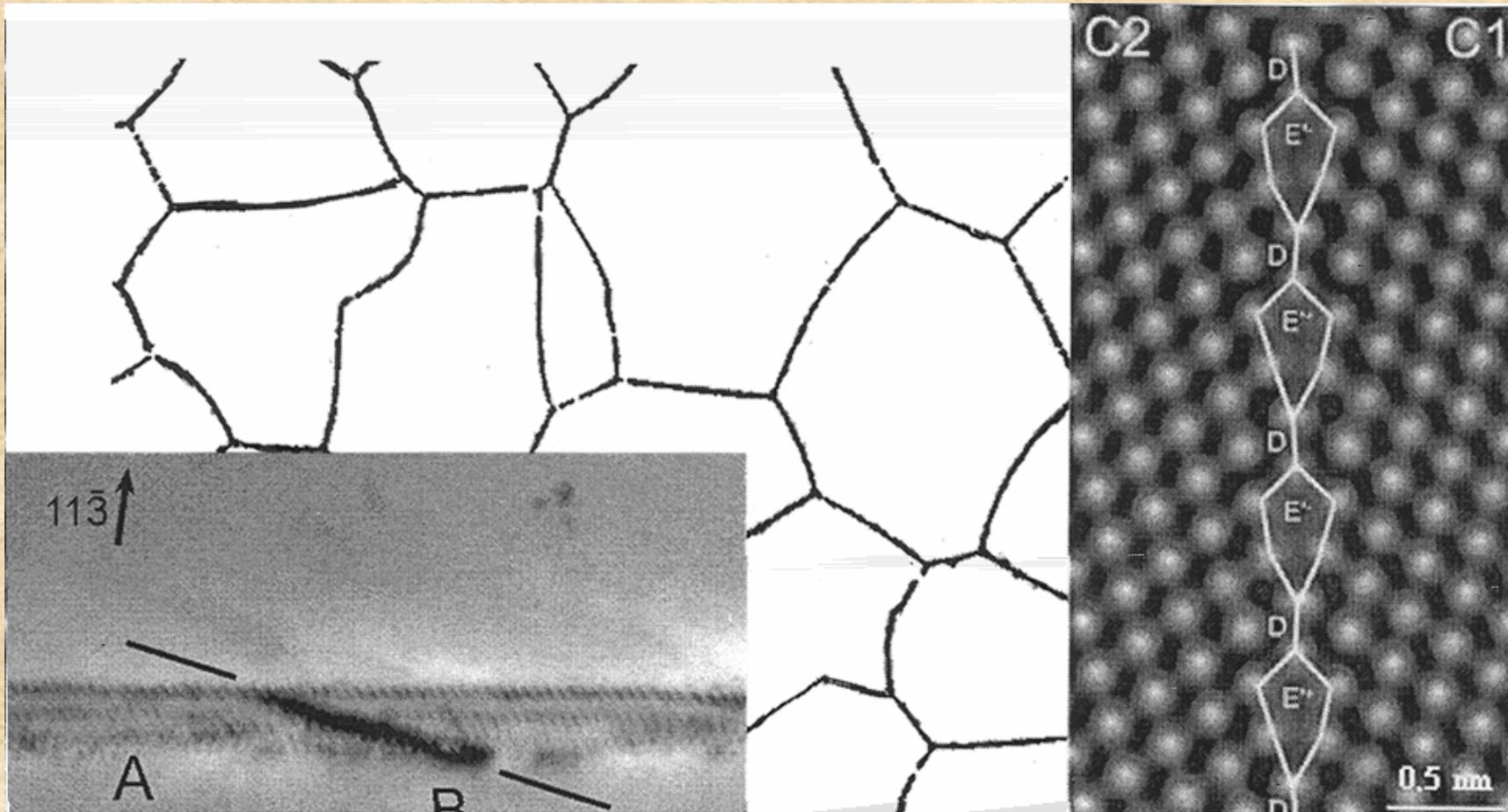
GRAIN BOUNDARY STRUCTURE and DEFECTS

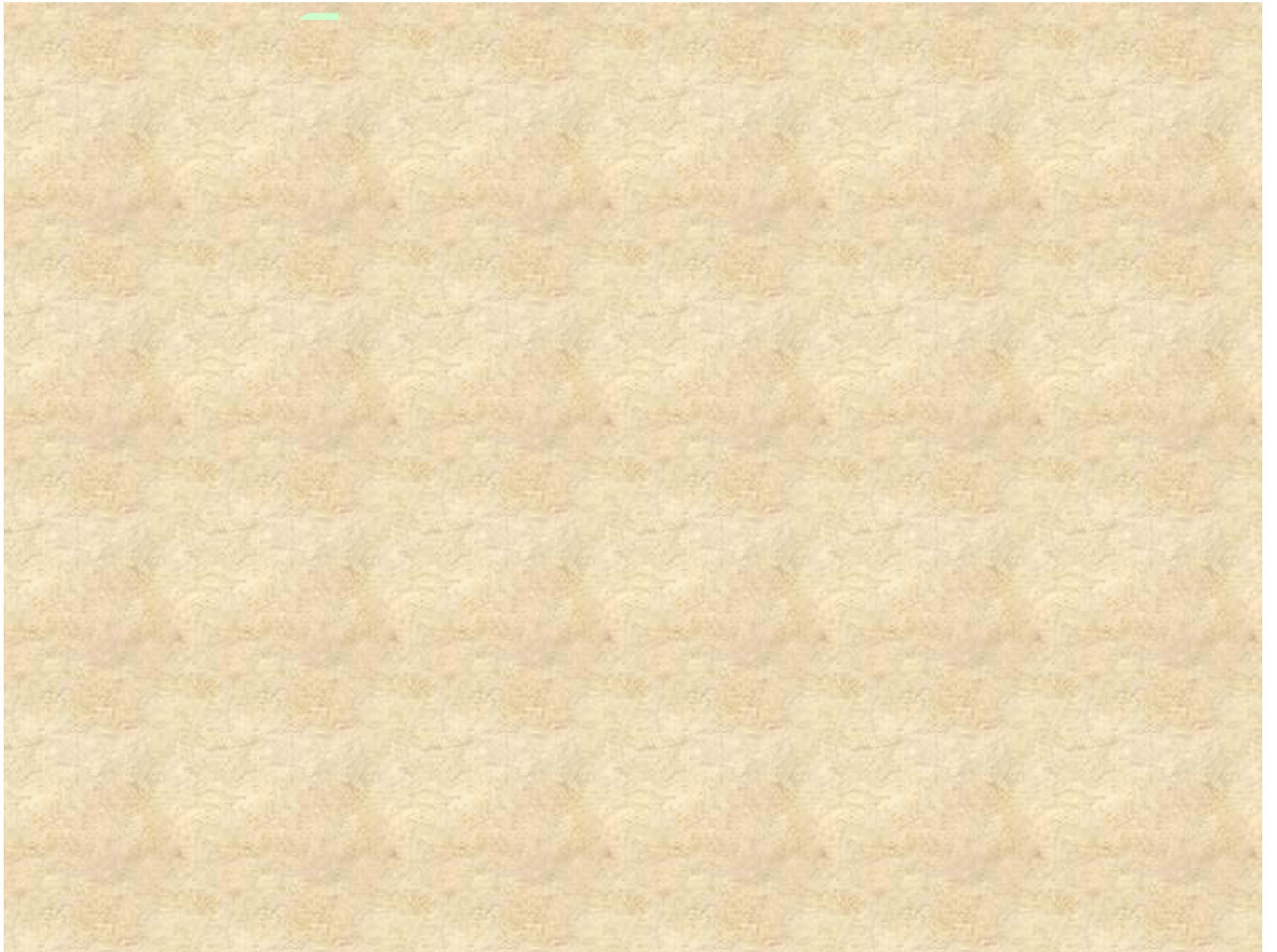
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1st Lecture Beijing
2008

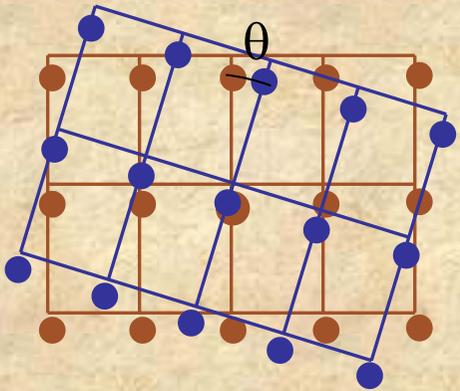
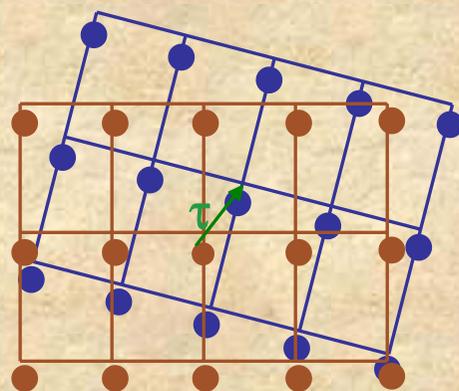
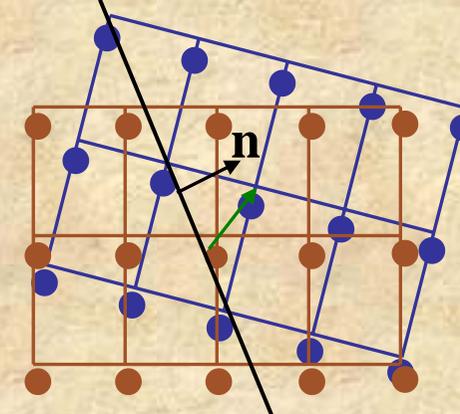
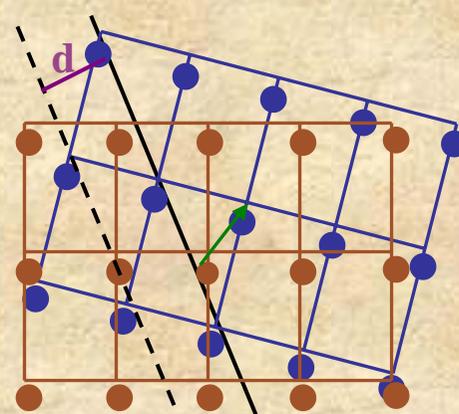
A GRAIN BOUNDARY at DIFFERENT SCALES





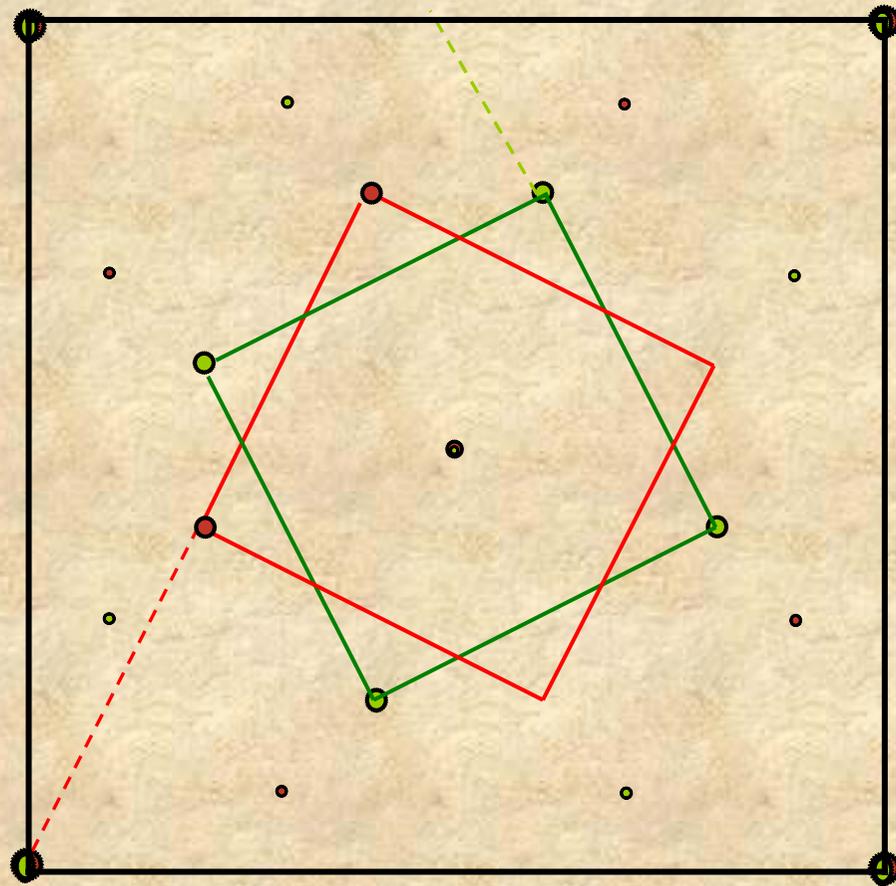
I) GEOMETRICAL ORDER: BICRYSTALLOGRAPHY

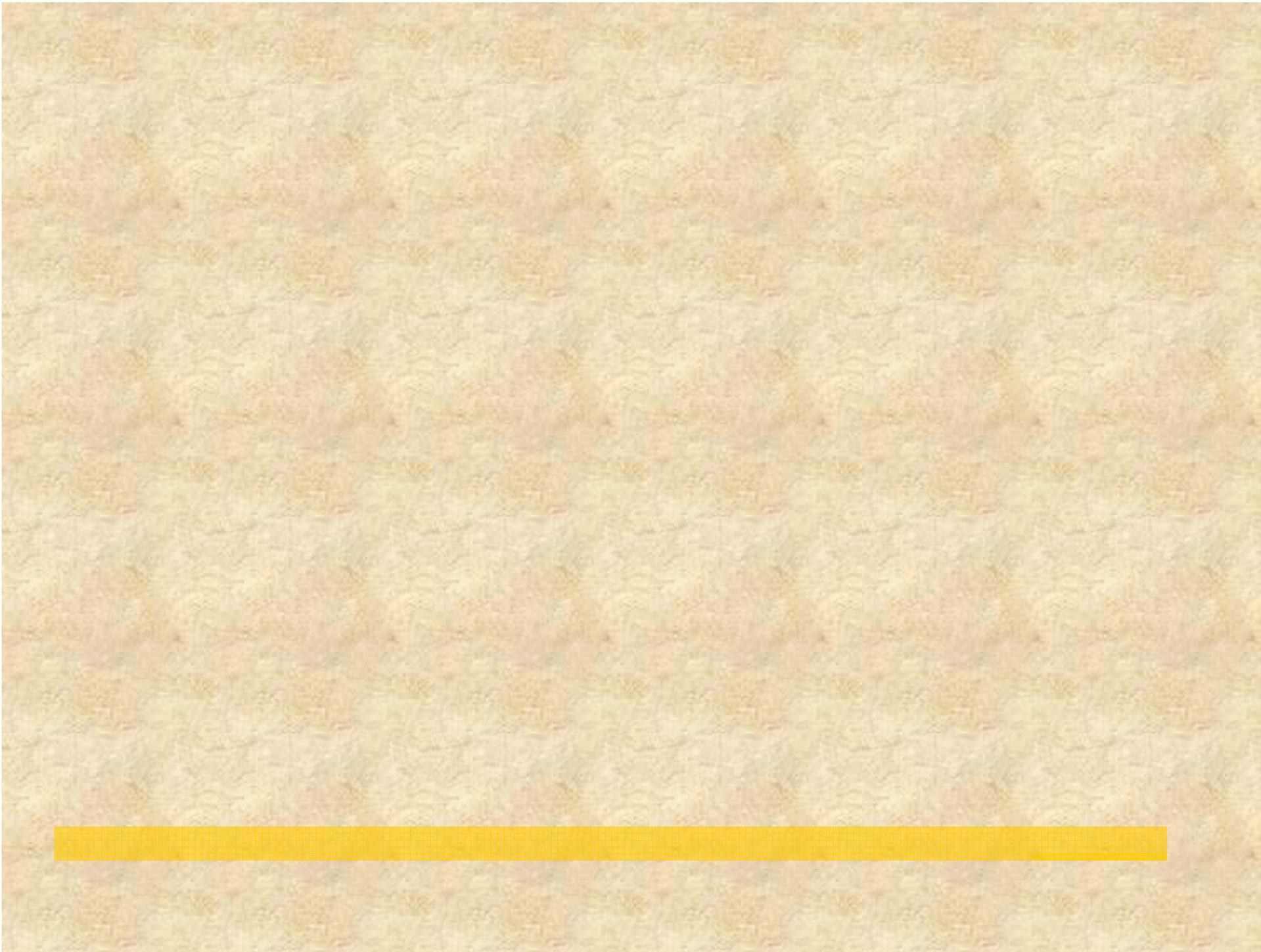
GEOMETRICAL PARAMETERS OF A GRAIN BOUNDARY

	Macroscopic	Microscopic
Interface operation (<i>bicrystal</i>)		
GB plane		
	<p>3 parameters for the rotation : θ $\langle uvw \rangle$</p> <p>+</p> <p>2 parameters for the plane orientation \mathbf{n}</p>	<p>3 parameters for the rigid translation τ</p> <p>+</p> <p>1 parameter for the plane position \mathbf{d}</p>

NOTION OF COINCIDENCE

CSL





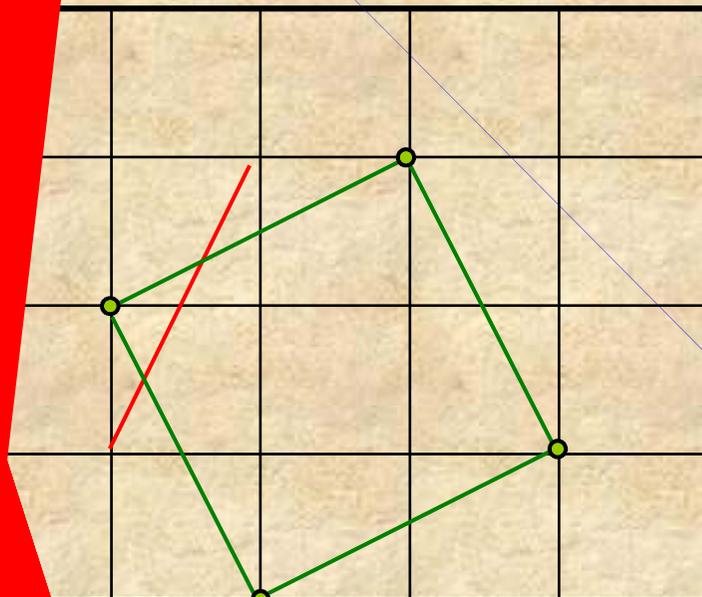
TRANSLATION LATTICE OF GRAIN BOUNDARY

Defines the Burgers vectors of perfect GB dislocations

DSC

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

$\infty \Rightarrow \mathbf{b}_{\text{DSC}}$



0 LATTICE

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

Fondamental equation

If $\boldsymbol{\tau} = \mathbf{0}$ (Bollmann)

$$\mathbf{x}_0 = \mathbf{R} \mathbf{x}_0 + \mathbf{B}_m$$

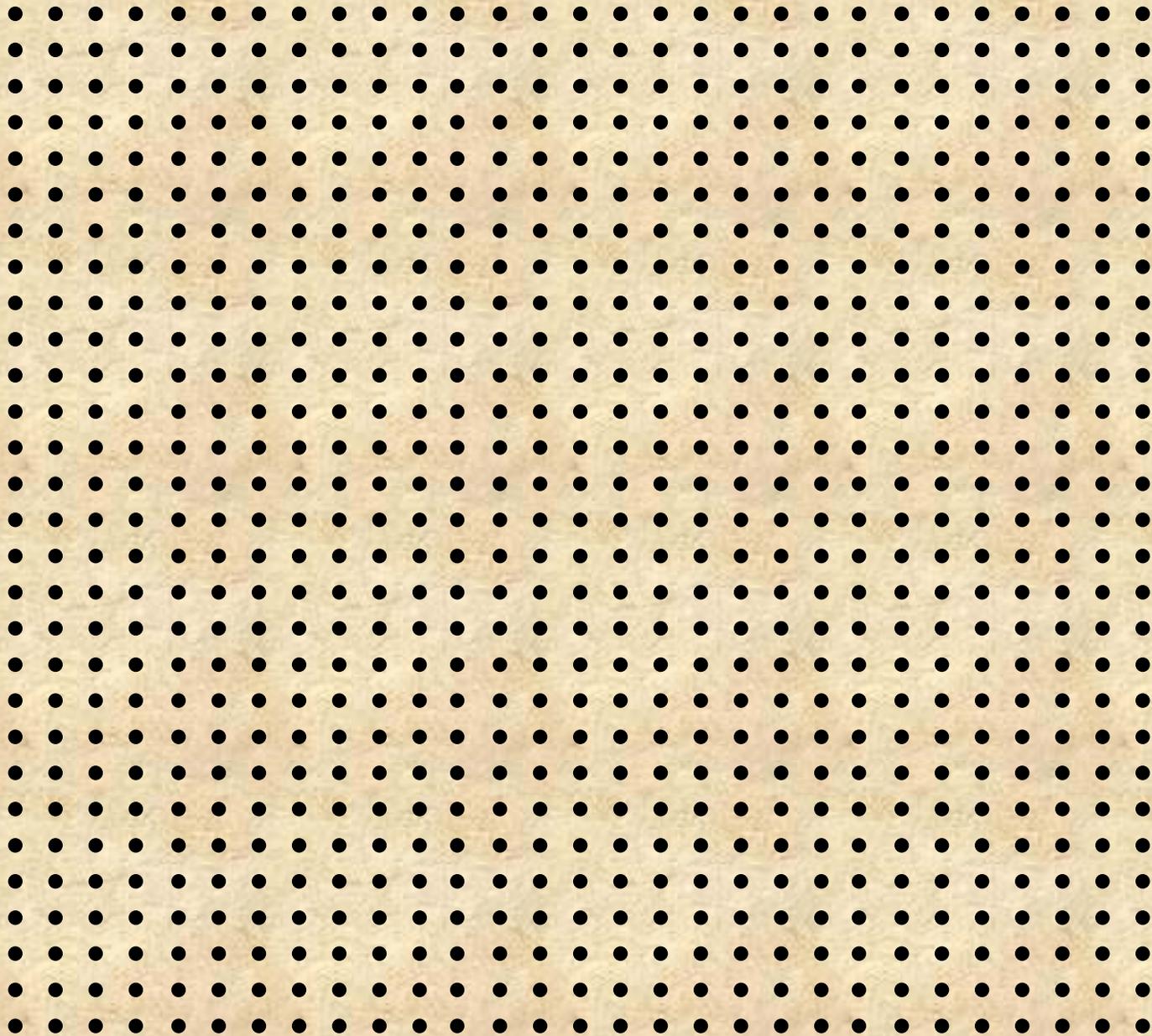
\mathbf{B}_m = translation vector in crystal

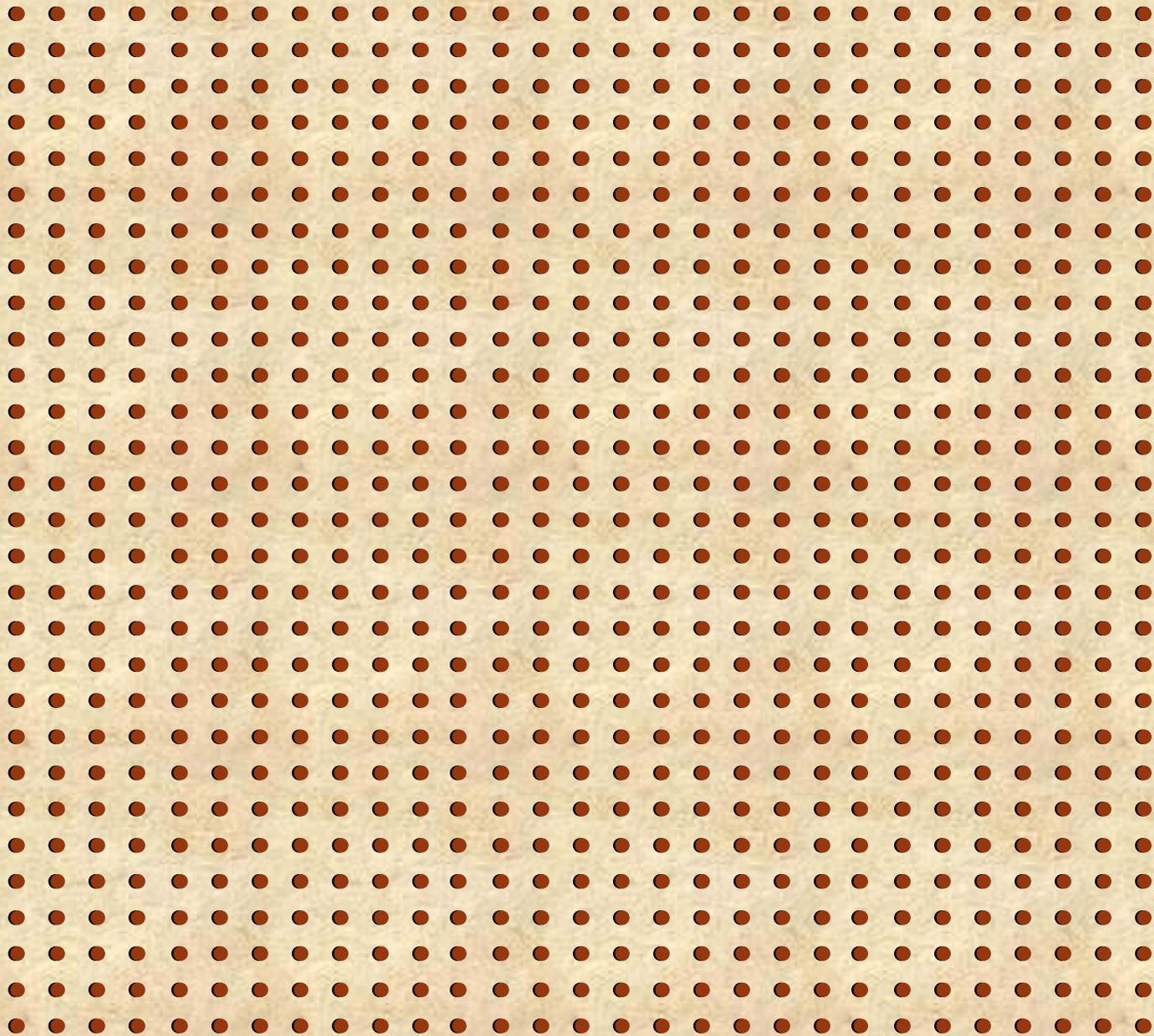
$$(\mathbf{I} - \mathbf{R}^{-1}) \mathbf{x}_0 = \mathbf{B}_m = \Sigma \mathbf{b}_m$$

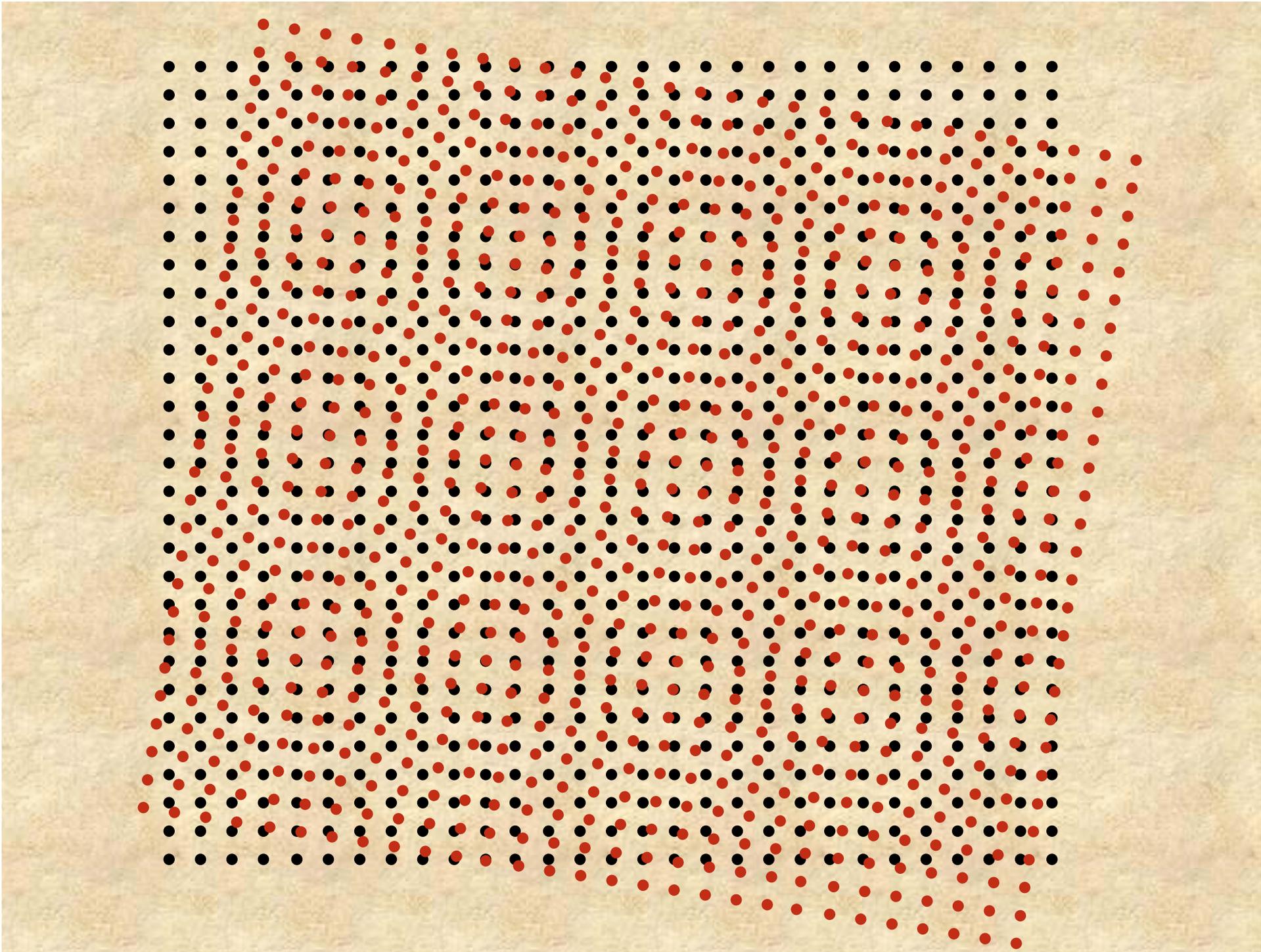
\mathbf{b}_m = Burgers vector for crystal

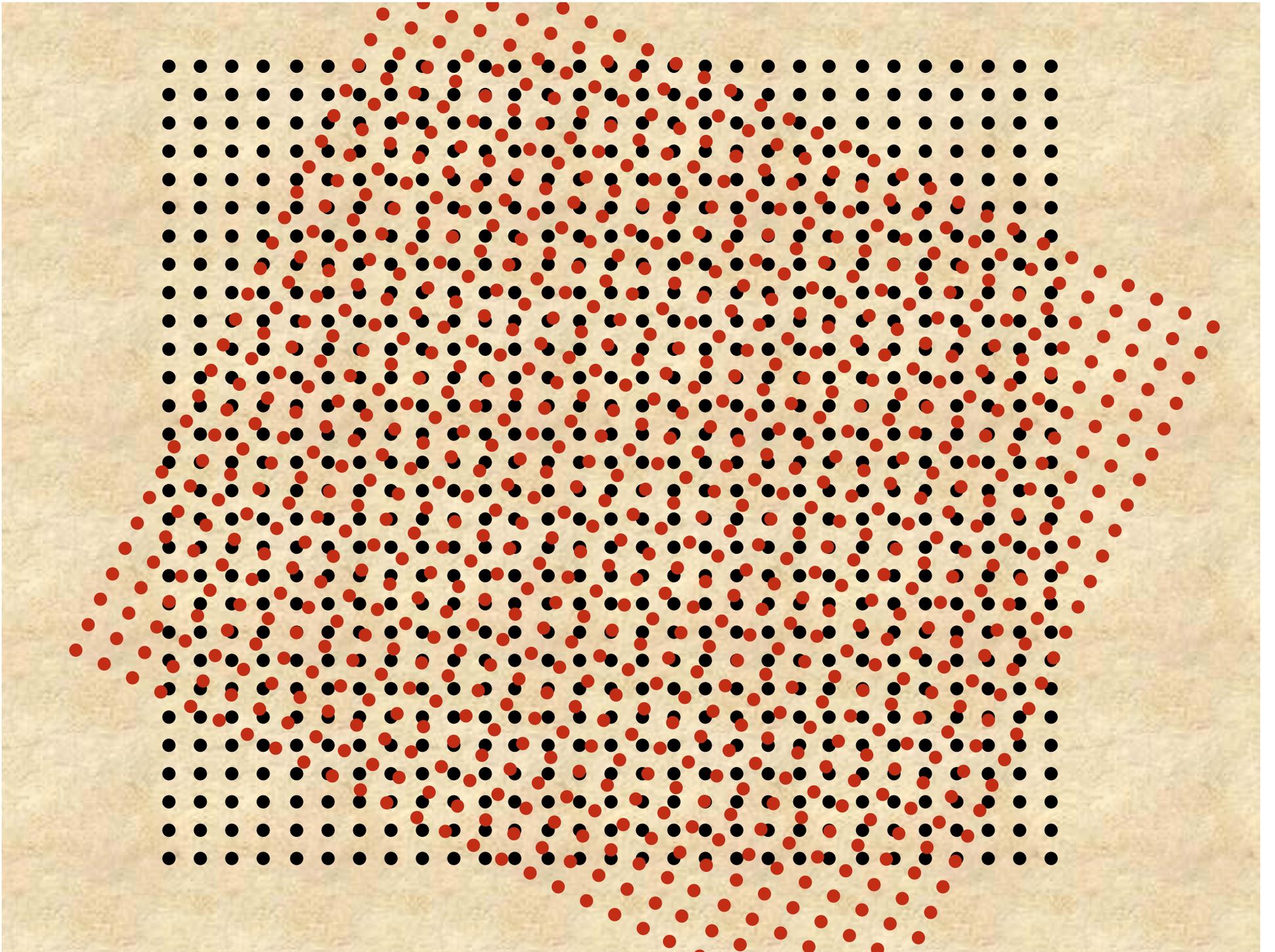
Properties

- Continuous function of the misorientation θ
- Any 0 point is an origine for the rotation

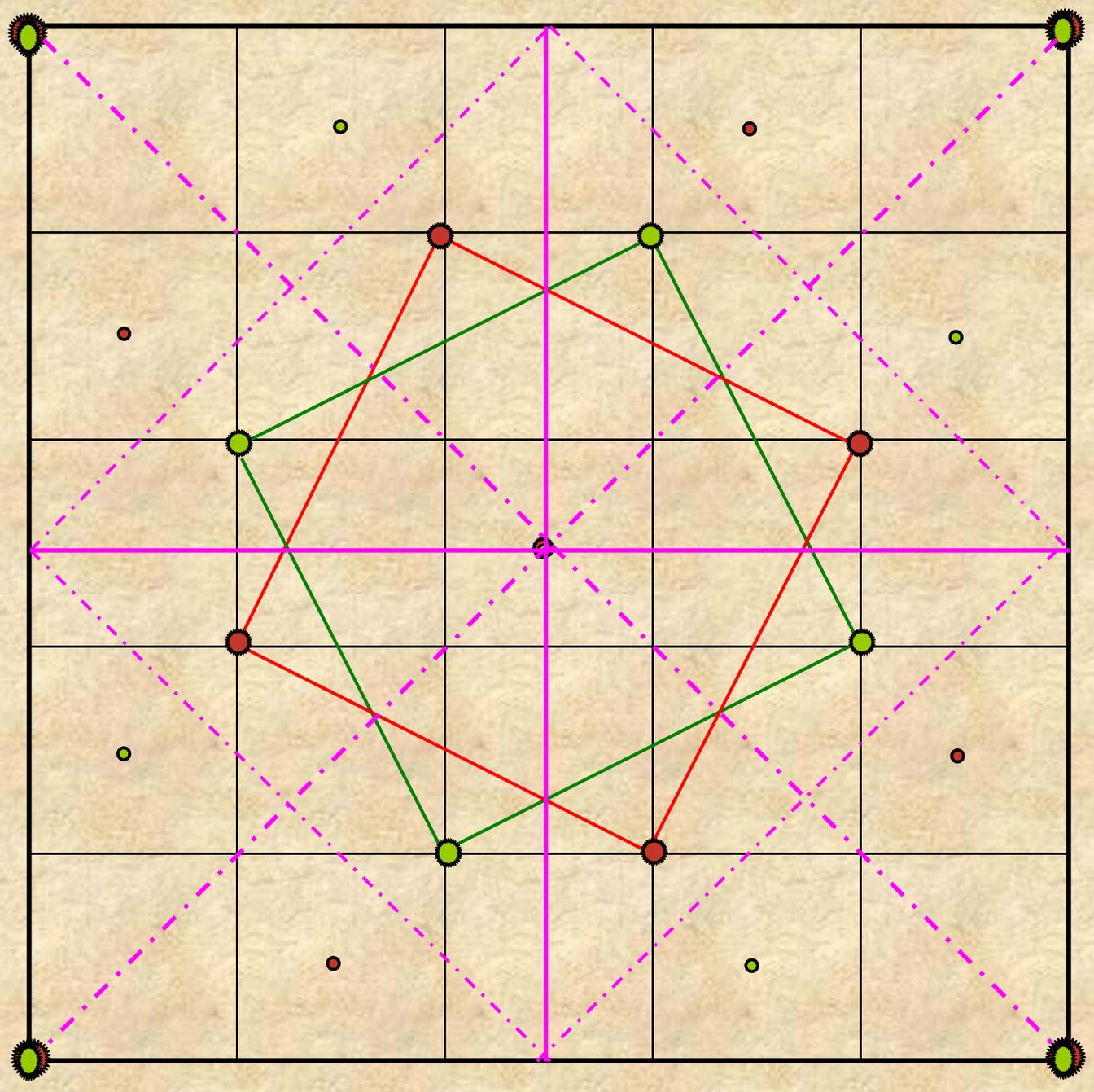




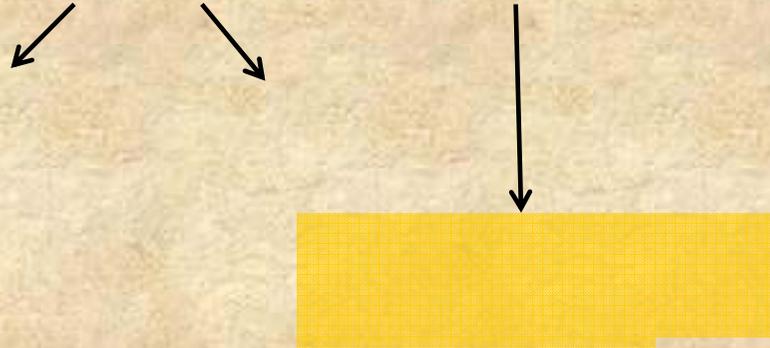




O Lattice
for Σ



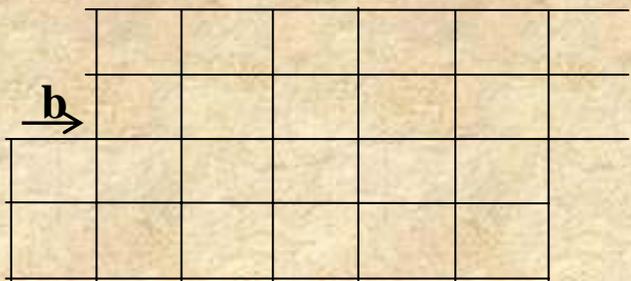
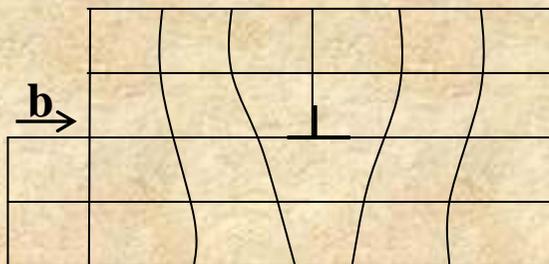
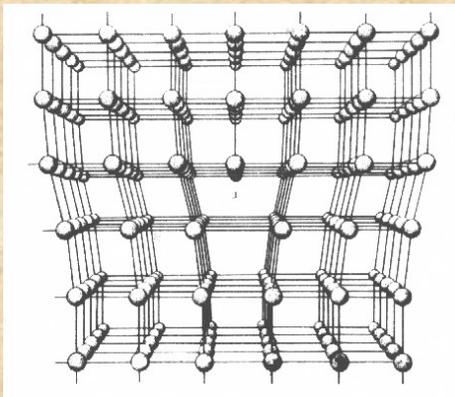
O₂ LATTICE



II) STRESS ORDER :
INTRINSIC DISLOCATIONS

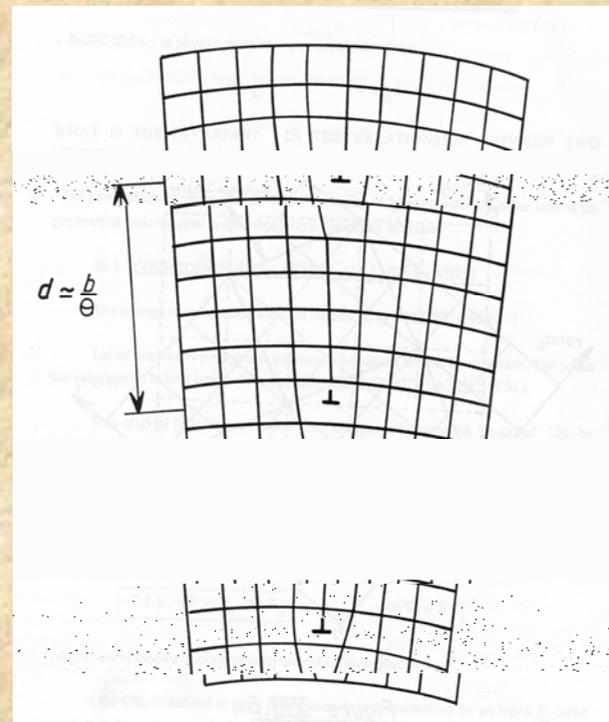
LINEAR and PLANAR DEFECTS

Dislocation



Elemental plastic deformation
 \mathbf{b} : translation lattice vector

Grain Boundary



Read and Shockley model

$$E_J = n E$$

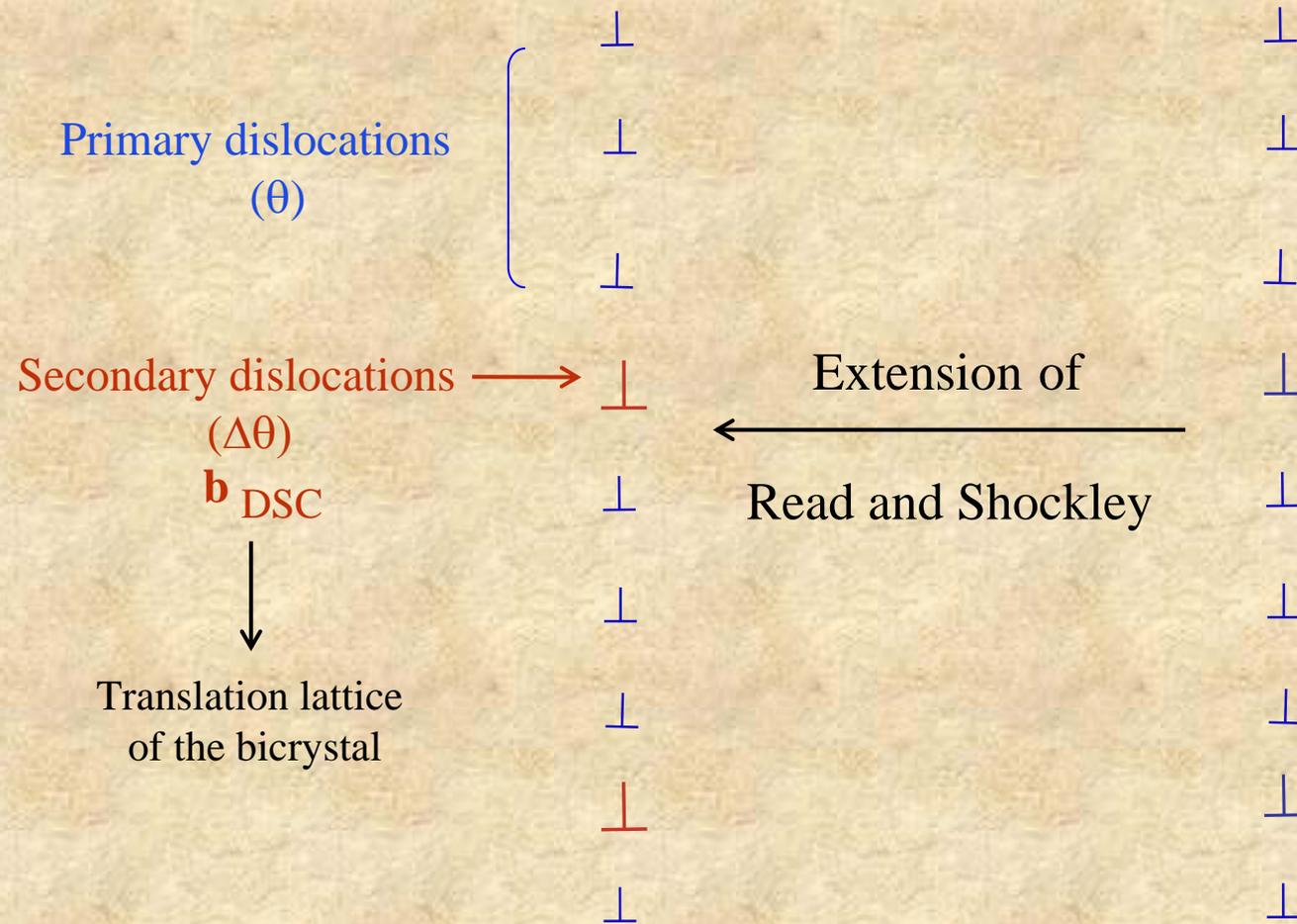
dislocation

\Rightarrow

$$E_J = E_0 \theta (A - \ln \theta)$$

The stress fields of neighbouring dislocations 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 \Rightarrow Points 0
- of the coincidence lattice \Rightarrow Points 02

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



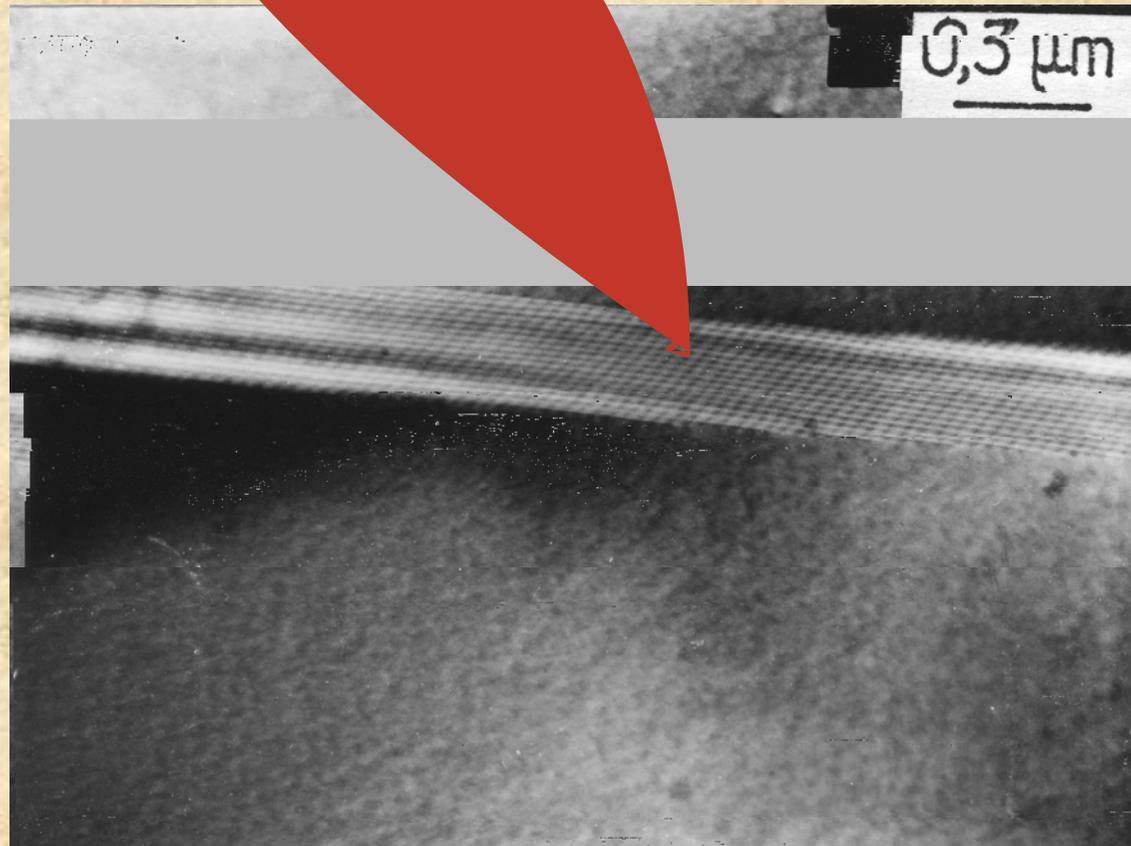
Intrinsic dislocations (**bad material**)

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

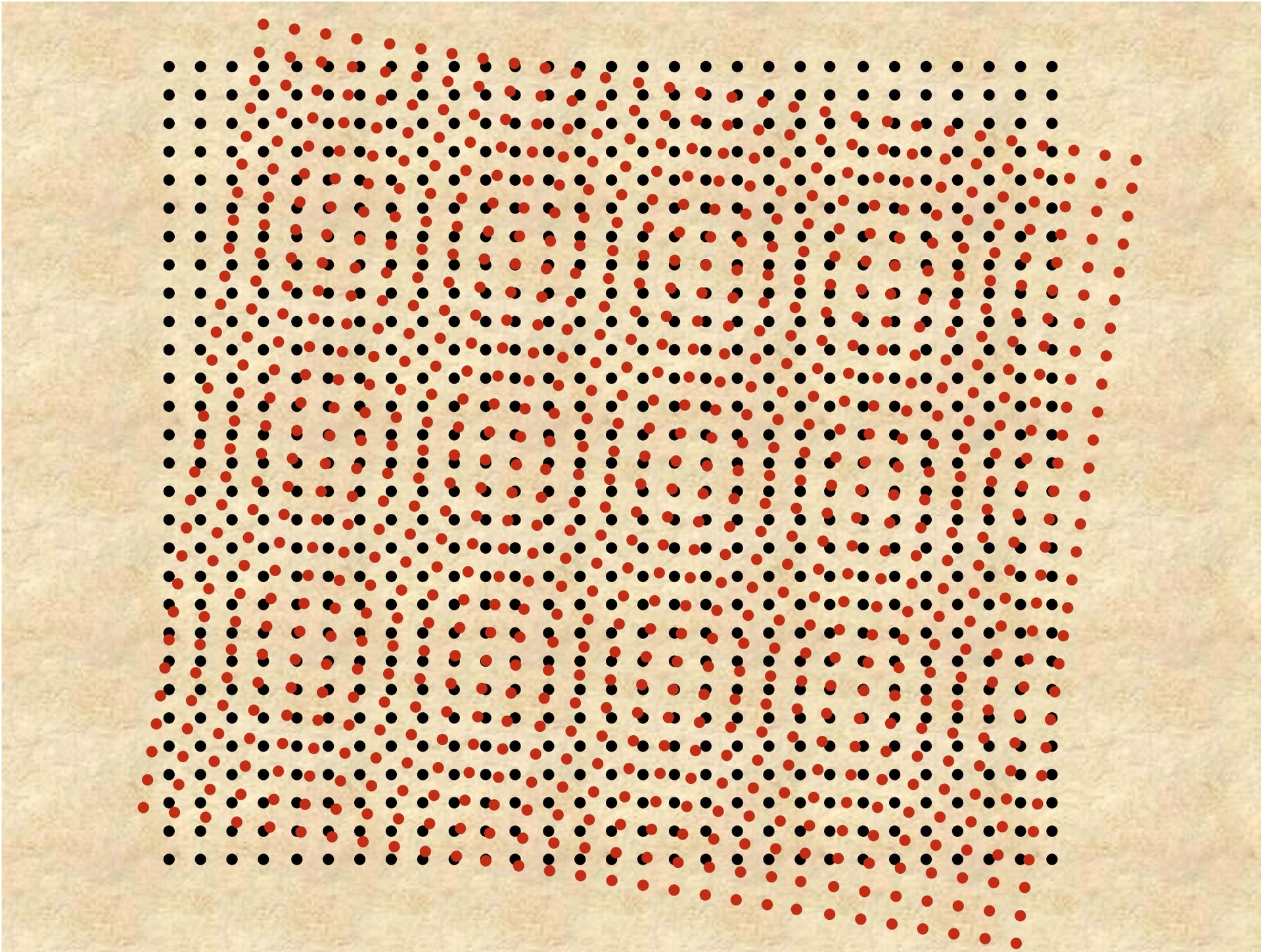
Primary intrinsic dislocations in a tilt GB

Material: Fe-0.2% C

GB: $\theta < 2^\circ$

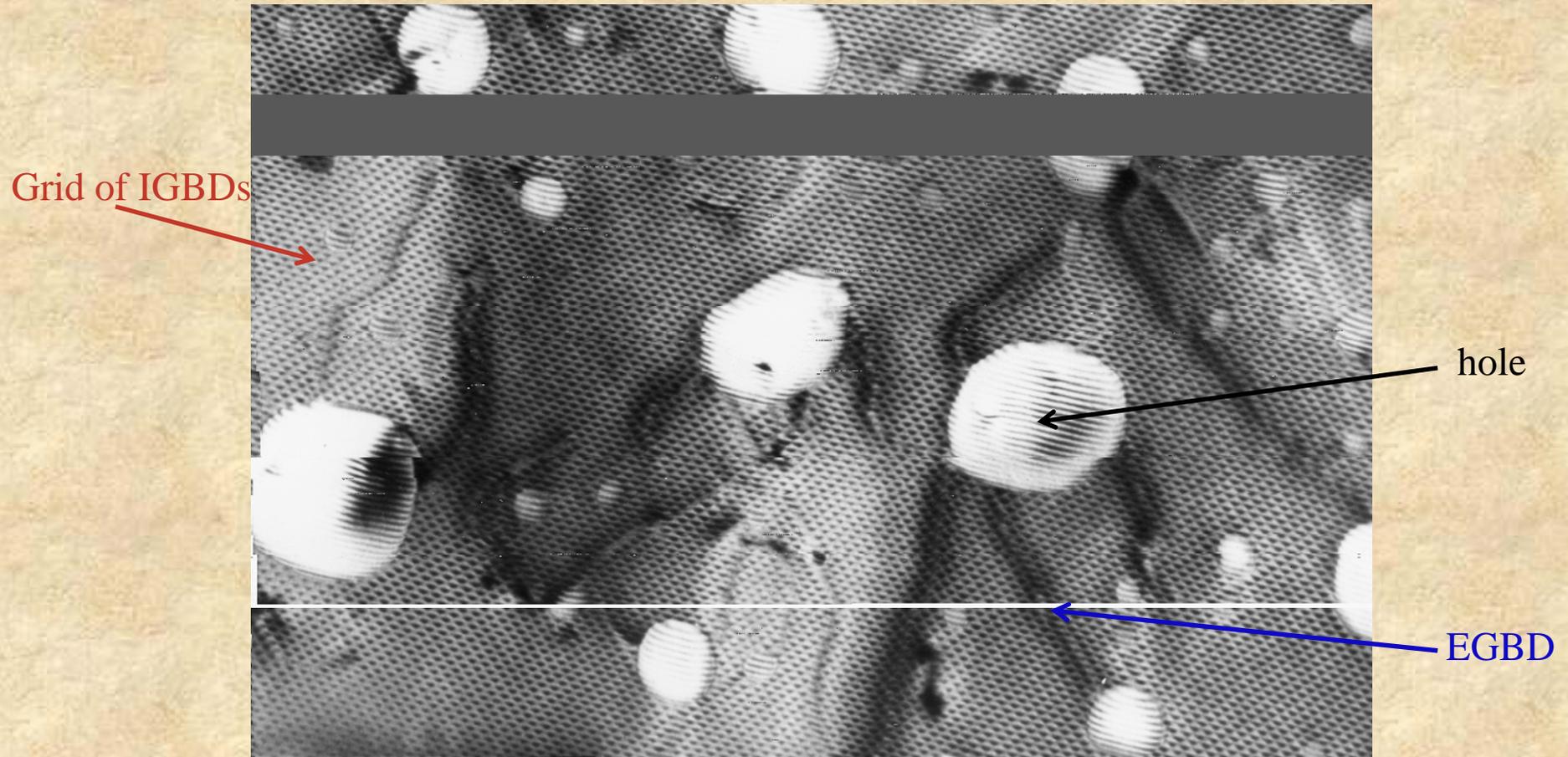


primary
Dislocations
network



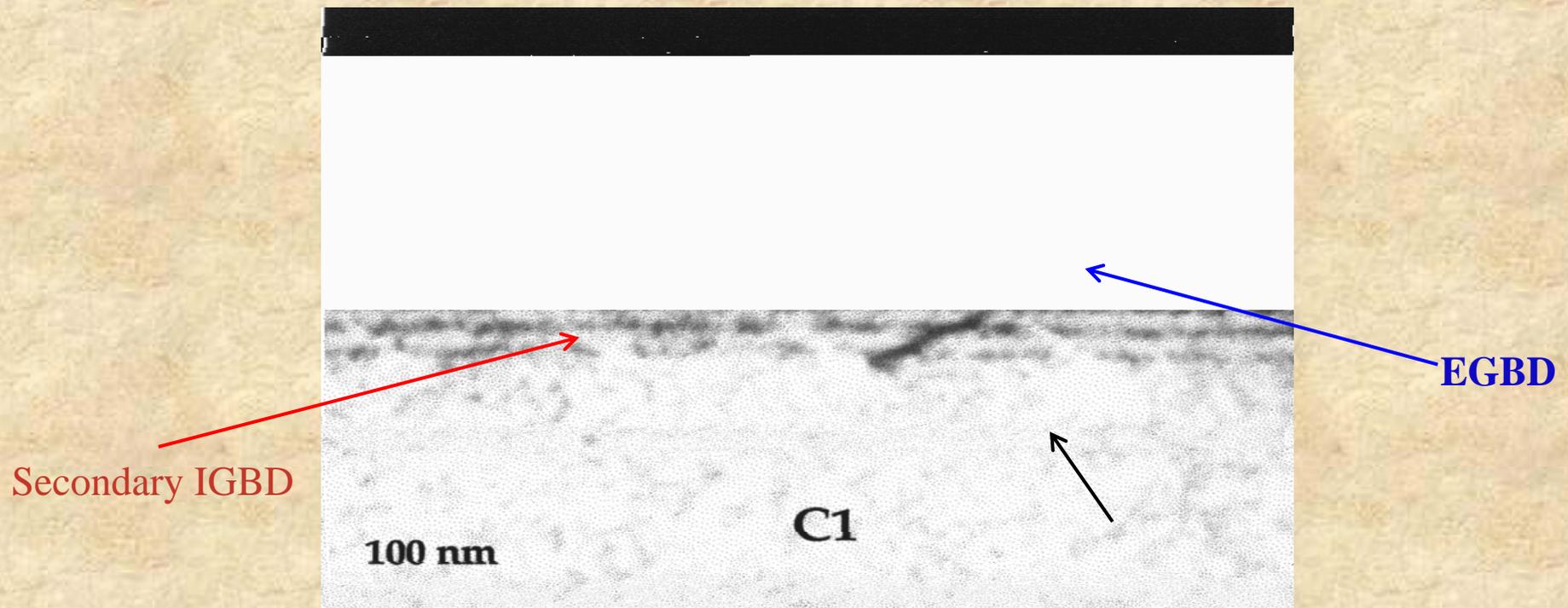
Example of primary intrinsic dislocations (IGBDs) in a twist GB

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



Example of secondary intrinsic dislocations (IGBDs)

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



INTRINSIC G.B. DISLOCATION MODEL SHORTCOMINGS

STRESS ORDER

⊥
⊥
⊥ } Primary

⊥ Secondary

BUT

⊥
⊥
⊥
⊥
⊥

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)

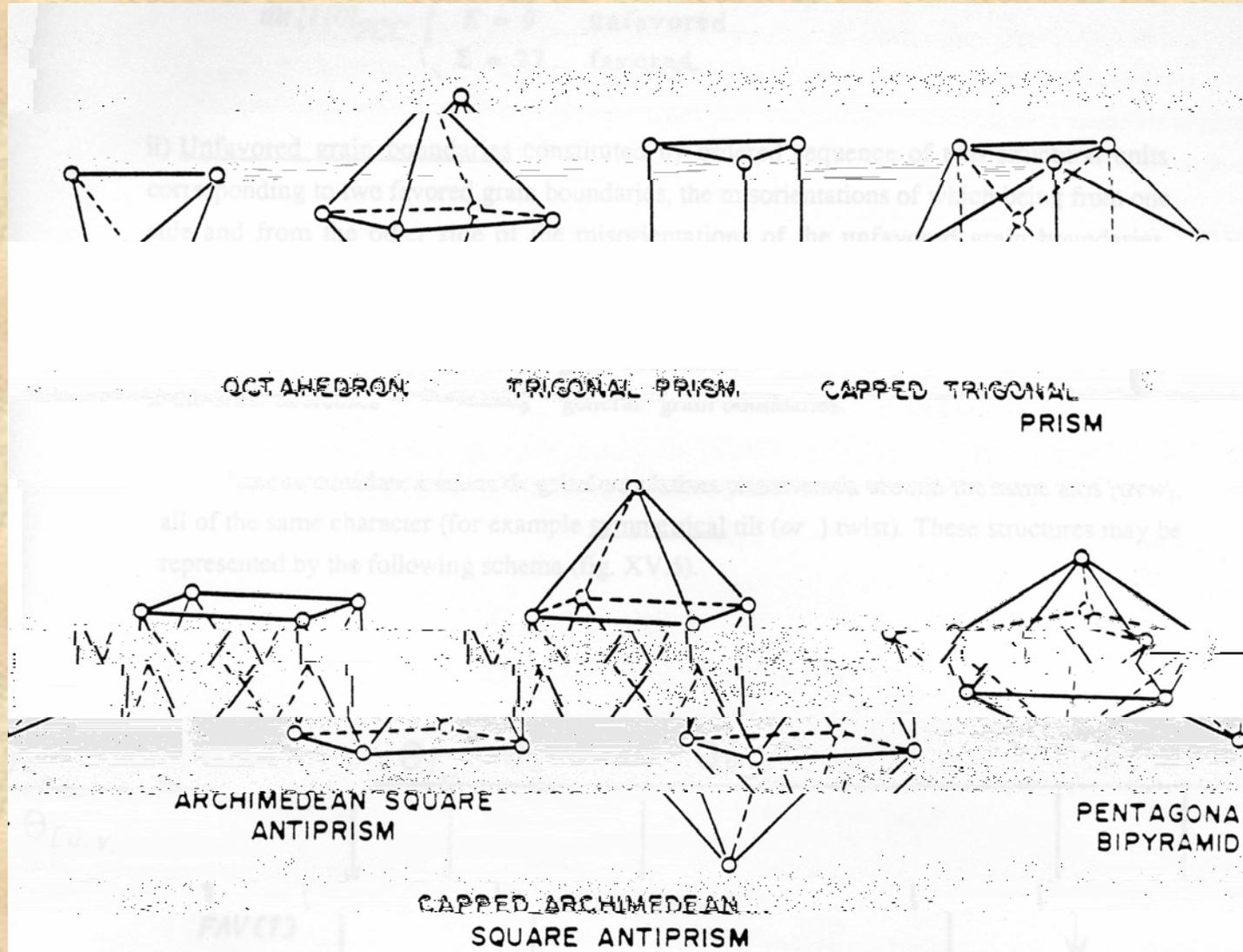
Energy by sites

⇒ Prevision of the interstitial and substitutional sites

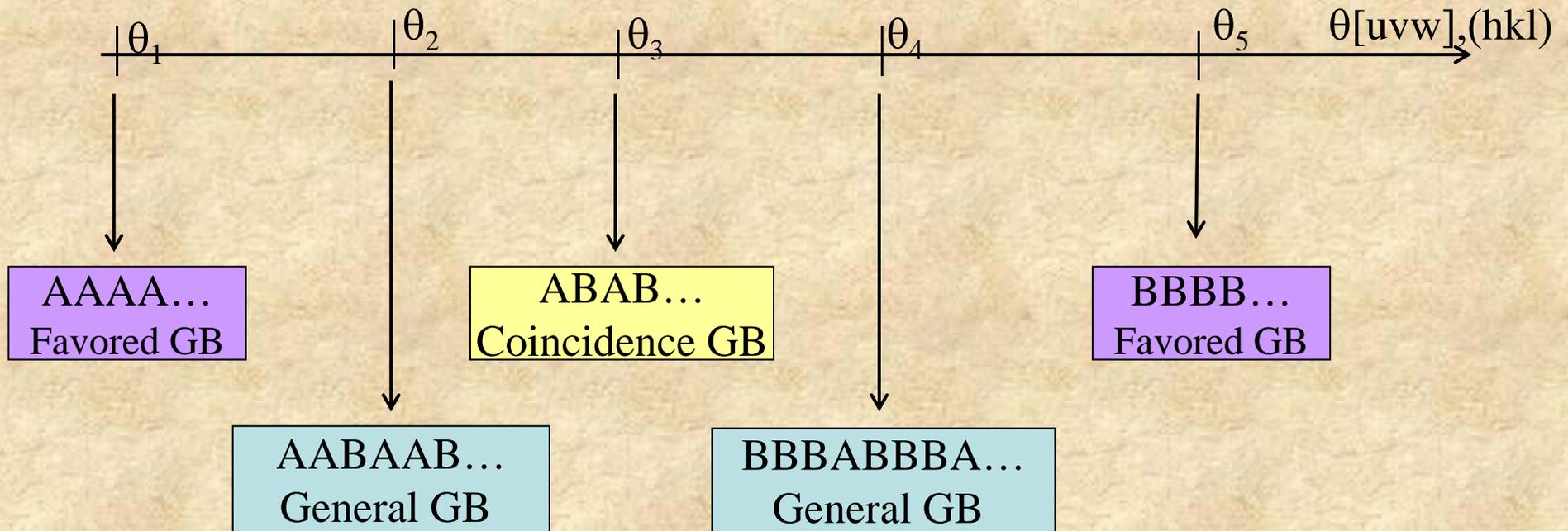


SEGREGATION

DIFFERENT STRUCTURAL UNITS FOUND IN GRAIN BOUNDARIES



ATOMIC ORDER : STRUCTURAL UNIT MODEL

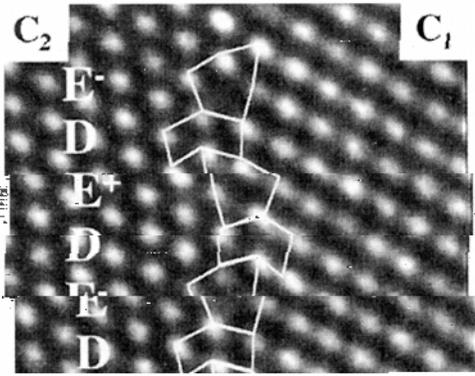


GB period : $\mathbf{p} = m \mathbf{u}_A + n \mathbf{u}_B$

simple principle **BUT COMPLEXITY**

- Distortion of the SUs
- Multiplicity of descriptions
- Hierarchy of descriptions

Description in terms of Structural Units (SU)



$\Sigma 9 \{221\}$ $\Sigma 11 \{332\}$ $\Sigma 3 \{111\}$

38° 94

50° 48

70° 53

$\theta <110>$

Intermediate GB

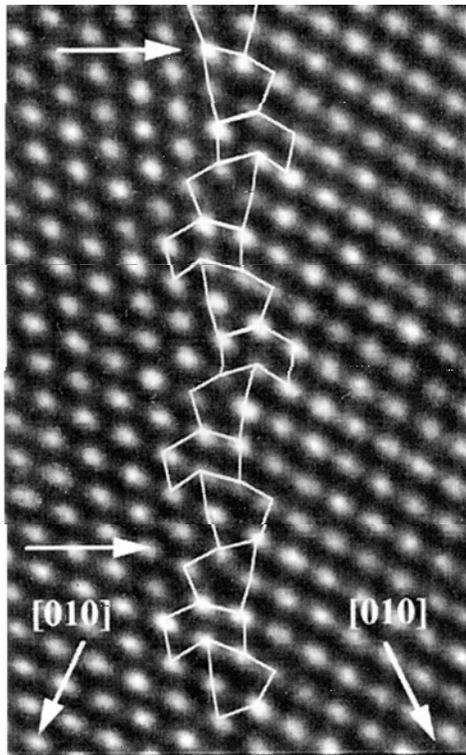
EEE...

Favored GB

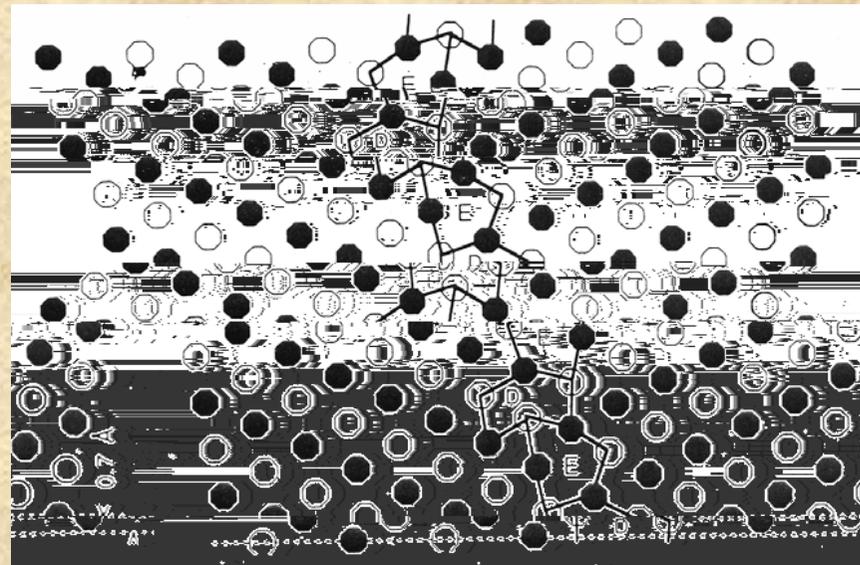
EDED...

DDD...

Favored GB

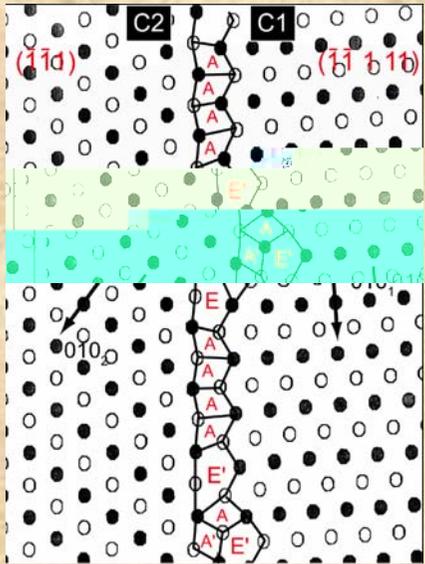
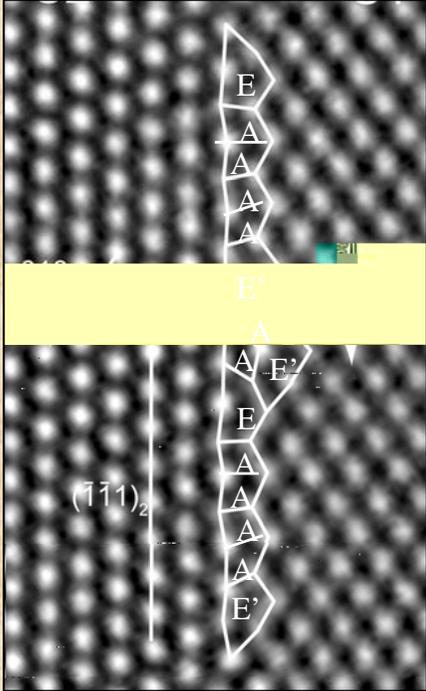
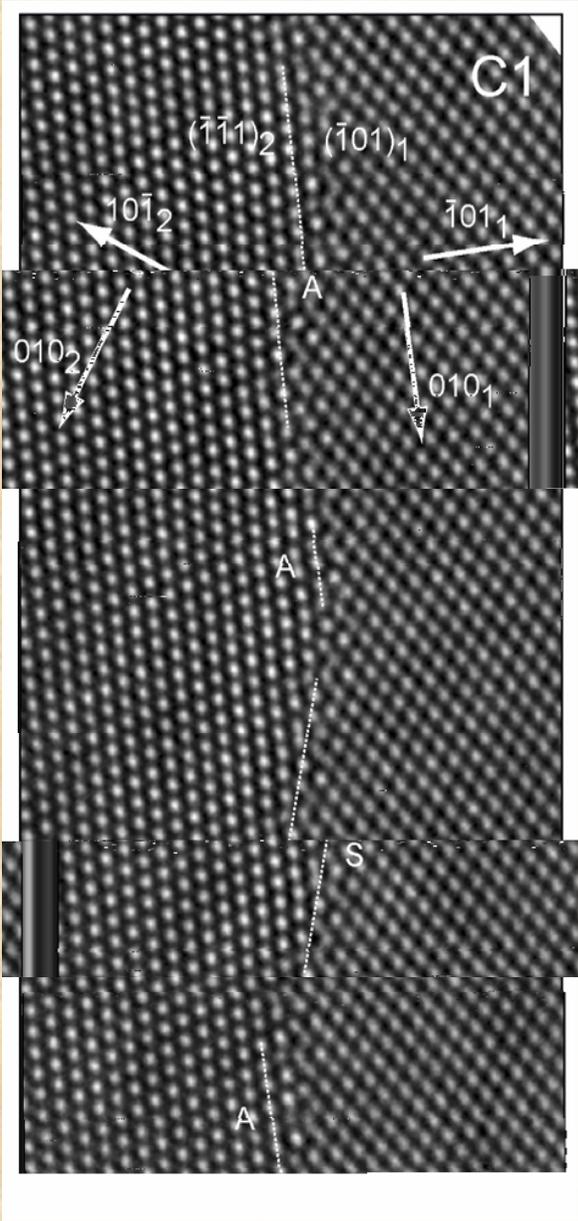


HRTEM image



Simulation

FACETING GB near $\Sigma 9$ in COPPER



STRUCTURAL UNITS/ INTRINSIC DISLOCATIONS

	⊥	A	
	⊥	A	
	⊥	A	
Secondary Dislocation	⊥	B	Minority unit
	⊥	A	
	⊥	A	
	⊥	A	
	⊥	B	
	⊥	A	



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: $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$

SHORTCOMINGS

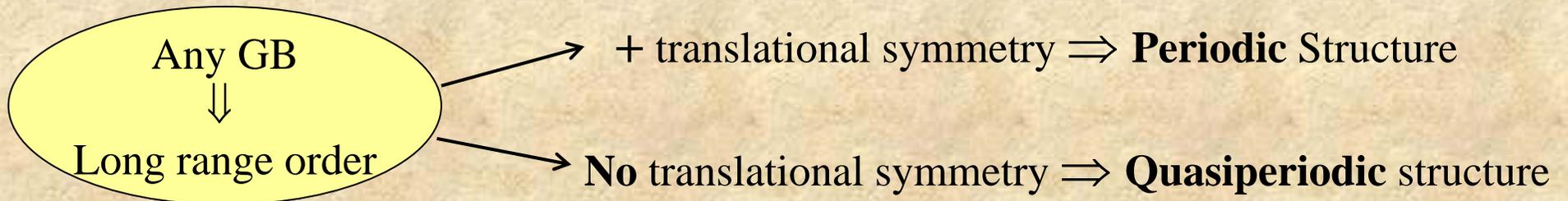
Geometry

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

Material

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

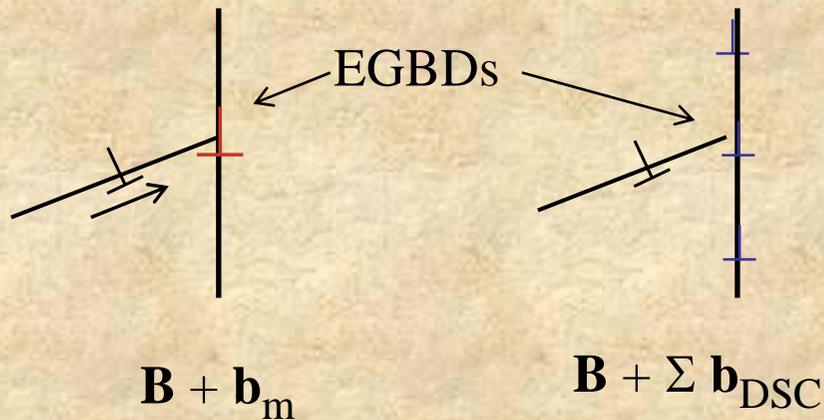
EXTENSION TO QUASICRYSTALLINE GBs



IV) GRAIN BOUNDARY DEFECTS EXTRINSIC DISLOCATIONS

GRAIN BOUNDARY EXTRINSIC DISLOCATIONS

Extrinsecus = from Outside



Towards equilibrium

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

$$R \Rightarrow R'$$

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

EXTRINSIC = NON EQUILIBRIUM \Rightarrow LONG RANGE STRESSES

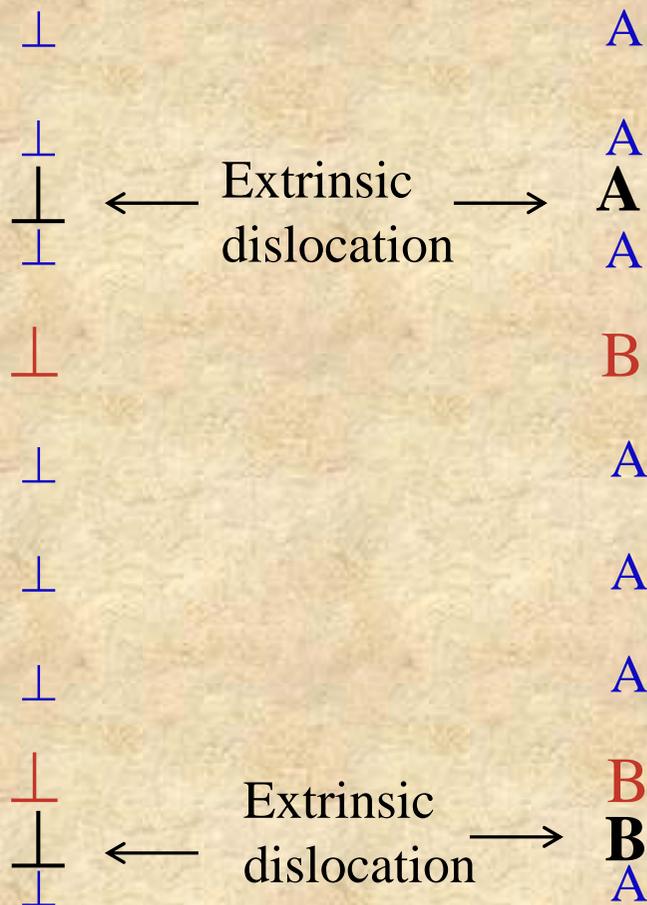


Accommodation

INTRINSIC = EQUILIBRIUM

\Rightarrow SHORT RANGE STRESSES

EXTRINSIC DISLOCATIONS/STRUCTURAL UNITS



Defect = Rupture of periodicity

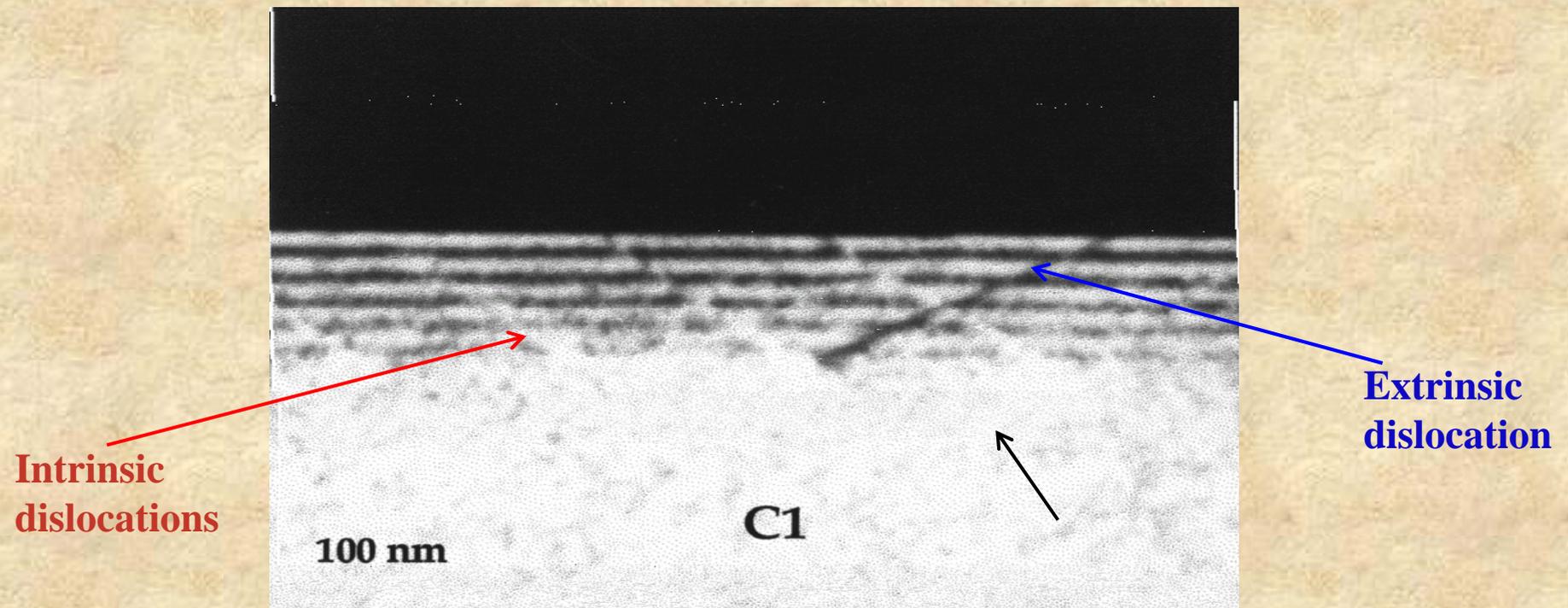
Addition or removal of one SU
≡ Extrinsic dislocation



b must be compatible with
the GB structure

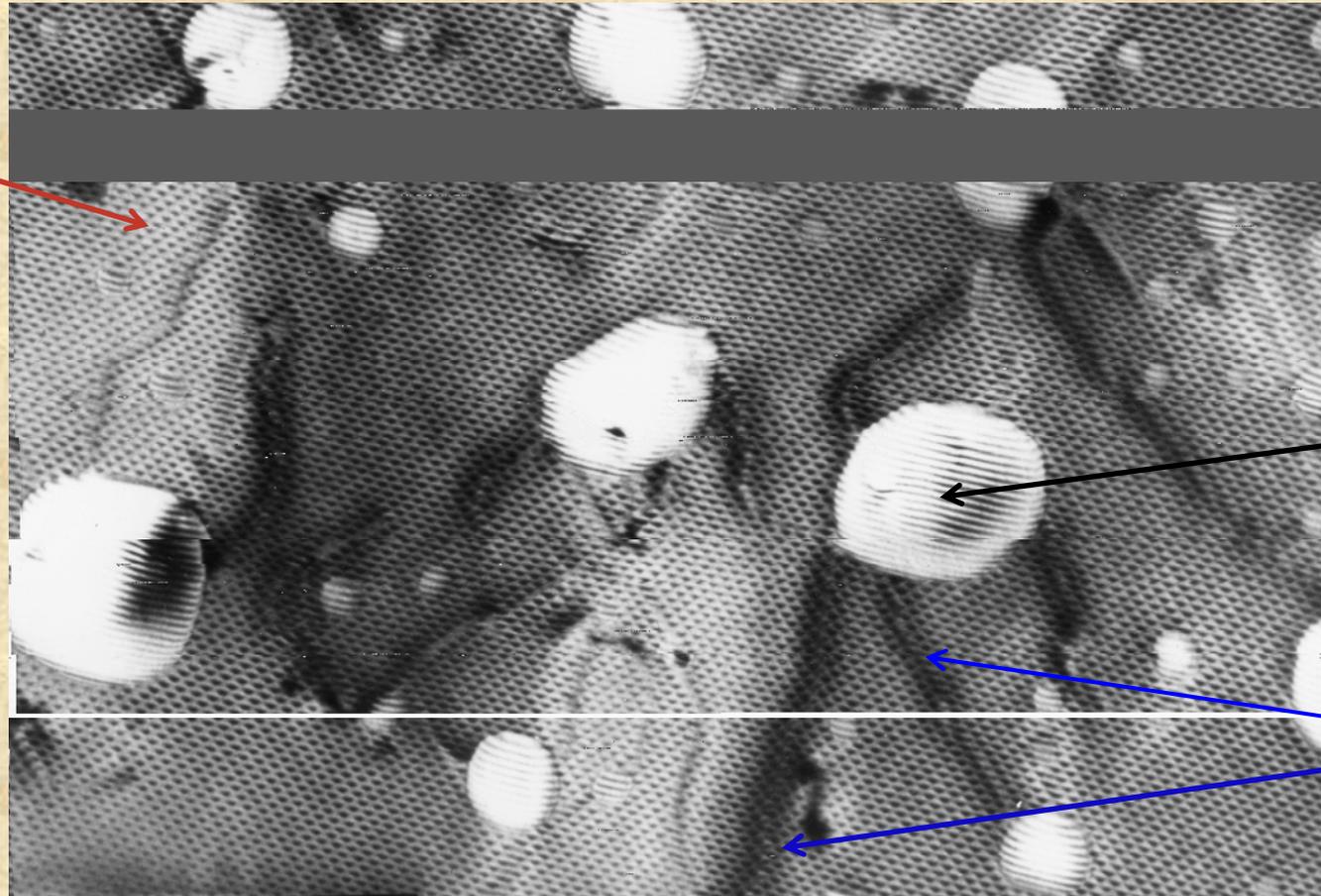
Example of Extrinsic Grain Boundary Dislocations (EGBDs) in a tilt GB

Near $\Sigma 3$ GB in copper



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

Intrinsic
dislocation
network



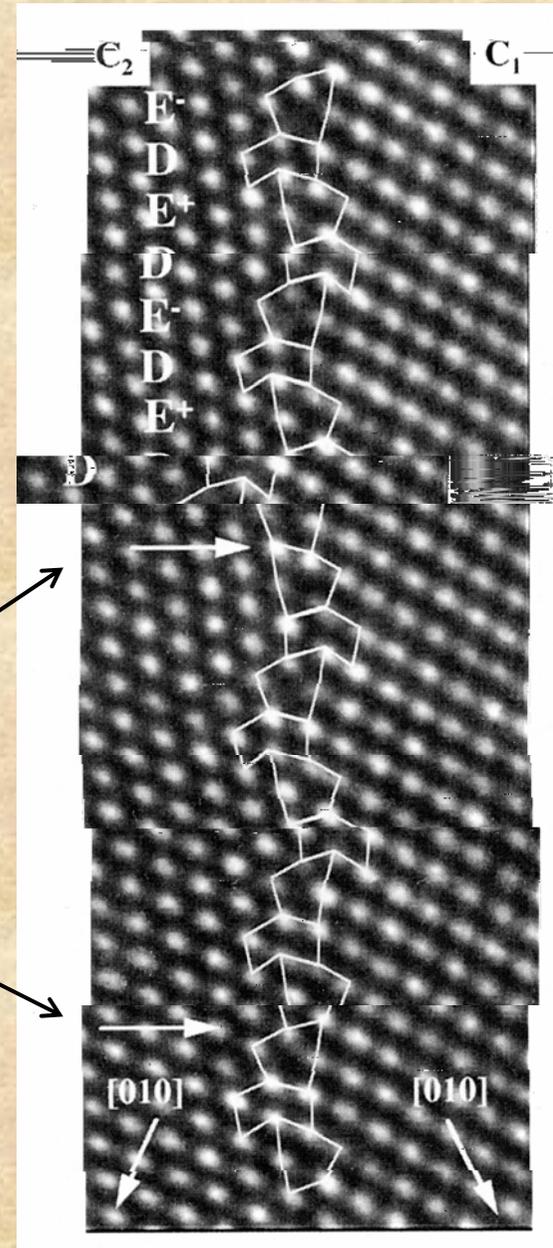
Hole

Extrinsic
dislocations

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

Example of EGBD/ SU in $\Sigma 11$ {332} in nickel

The absence of a $\Sigma 3$ SU corresponds to the presence of a sessile EGBD with $b_{\text{DSC}} = a/22 \langle 323 \rangle$



EQUILIBRIUM / NON EQUILIBRIUM

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

*** Second lecture**