INTERNATIONAL ATOMIC ENERGY AGENCY
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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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SMR.550 - 27

SPRING COLLEGE IN MATERIALS SCIENCE ON "NUCLEATION, GROWTH AND SEGREGATION IN MATERIALS SCIENCE AND ENGINEERING"

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TRANSPORT PROCESSES (INCLUDING RADIATION ENHANCED DIFFUSION)

Part V

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Self-Organization in Solids

by

Anisotropic Transport of Matter

or

Formation of Ordered Defect Structures in Solids far away from Thermal Equilibrium

Structures occur in nature on all size scales:

(i) gallactical structures

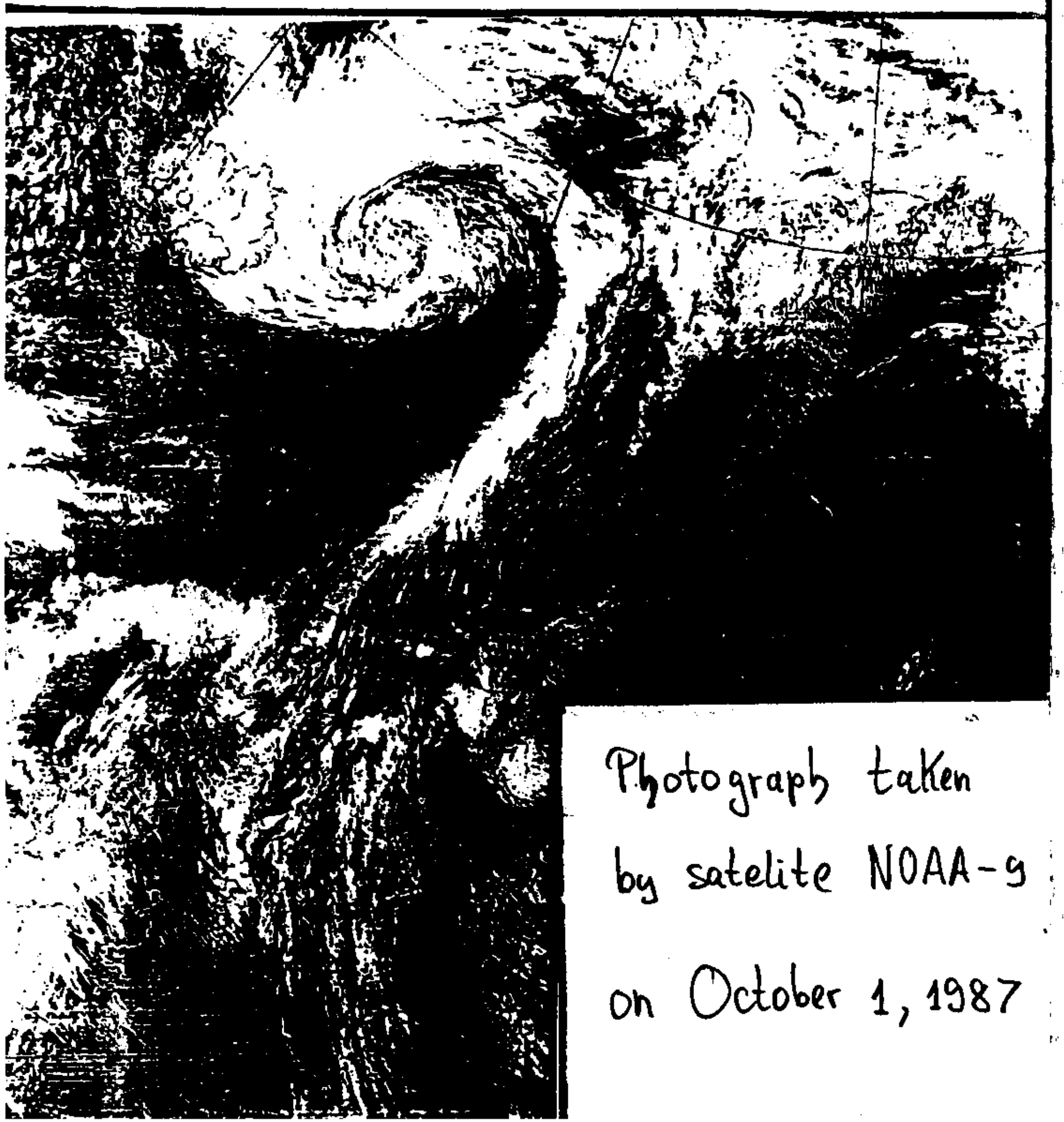
(ii) global structures (see next transparency)

(iii) macroscopic structures (e.g., waves on the ocean, ripples in the sand)

(iv) mesoscopic structures (5 nm ... 500 nm)

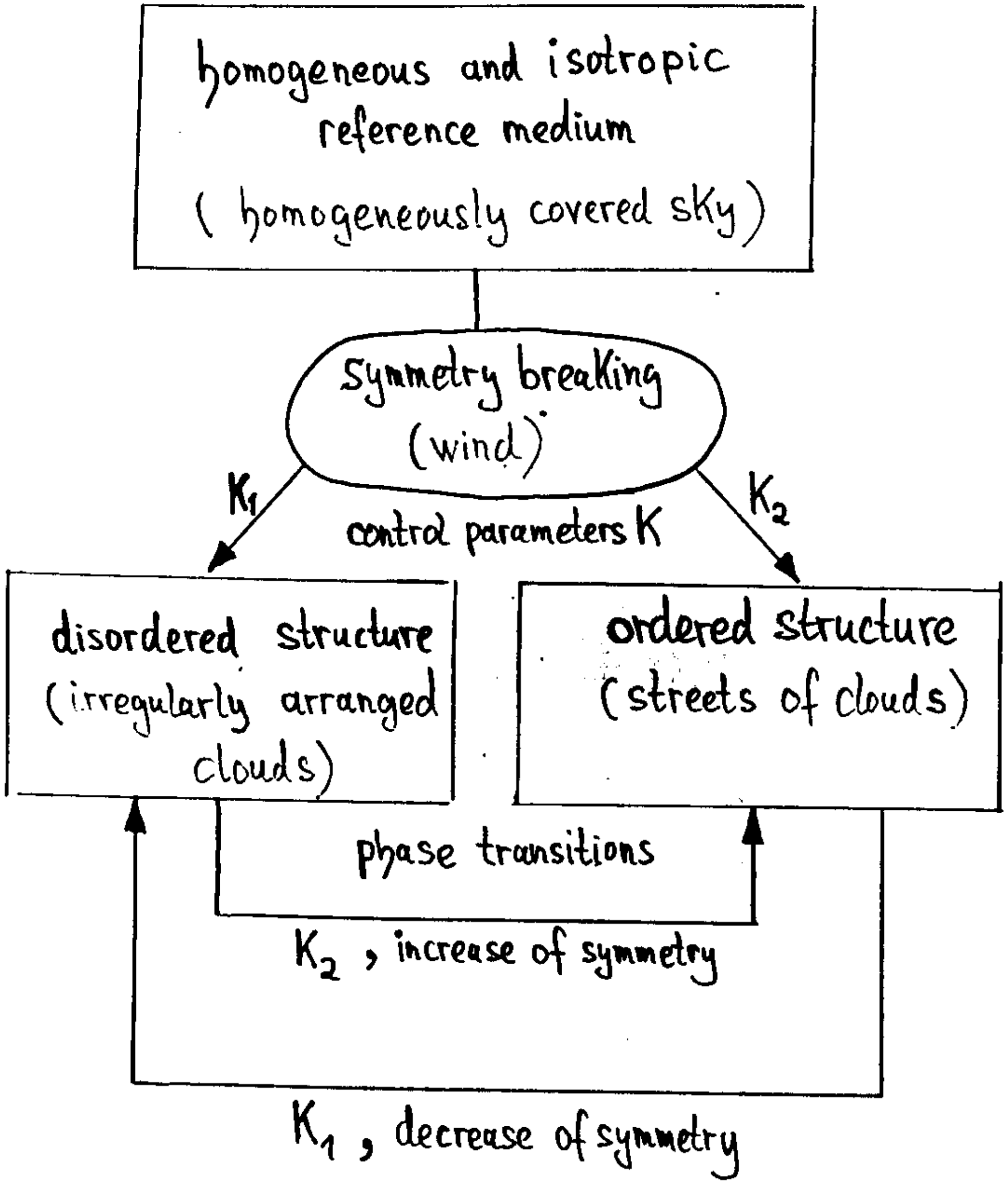
(v) microscopic structures (e.g., crystal lattices)

Swirl of clouds (northwest of Scandinavia) — an example of a structure on the global scale



Photograph taken by satelite NOAA-9 on October 1, 1987

What is a (spatial) ordered structure?



Ordered Structures in Thermo= dynamic Equilibrium

$$F \equiv U - TS = \text{minimum} \qquad T, V = \text{const}$$

F: free energy; U: internal energy; S: entropy (disorder)

How can ordered structures be produced?

High T → high U → high S

gas (molecular disorder)

Low T : $S \to 0$ (3rd law)

→ U = minimum

ordered structures

crystalline solids (microscopic order)

vortex lattices (mesoscopic order)

Ordered Structures far from Equilibrium

Prerequisite for formation of order:

$$dS = dS_{in} + dS_{ex} < 0$$

$$dS_{in} > 0 \quad (2^{nd} \text{ law})$$

→ $dS_{ex} < 0 \;, \; |dS_{ex}| > dS_{in}$

→ **dissipative systems**

Examples

1) Explosion?

2) Undercooling of a melt

- rapid export of heat
- symmetry breaking, since rate of crystallization depends on crystallo= graphic directions

D1 dentrites (conditionally ordered structure)

(Quasi-) Steady States

(1) open systems

(2) far away from equilibrium

(3) strongly non-linear

(4) symmetry breaking (by external boundary conditions or internal constraints)

(5) suitable values of the control parameters (bifurcation):

unstable homogeneous / disordered phase

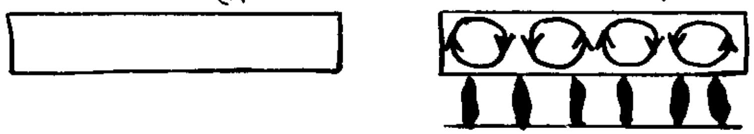
↓ fluctuations ↓

stable ordered structure

Examples

1) Laser (Haken)

2) Bénard-type structures in liquids:



Great advantage of structures in solid: metastabl

Ordered Structures in Solid Matter

D2 Dislocation pattern in a cyclically deformed Cu single crystal (room temperature, $\hat{\varepsilon} = 10^{-4} \dots 10^{-2}$)

D3 Periodically arranged walls of defect clusters $\parallel \{100\}$ in p^+-irradiated Cu ($\lesssim 100°C$, 3.4 MeV, 0.65 dpa)

D4 Krypton bubble lattice $\parallel \{0001\}$ in Kr^+-implanted α-Zr (400°C)

D5 Lattice of stacking-fault tetrahedra in e^--irradiated Ag (primitive-cubic $\parallel$ fcc host lattice, room temperature, $6.3 \times 10^{27}\ e^-/m^2$)

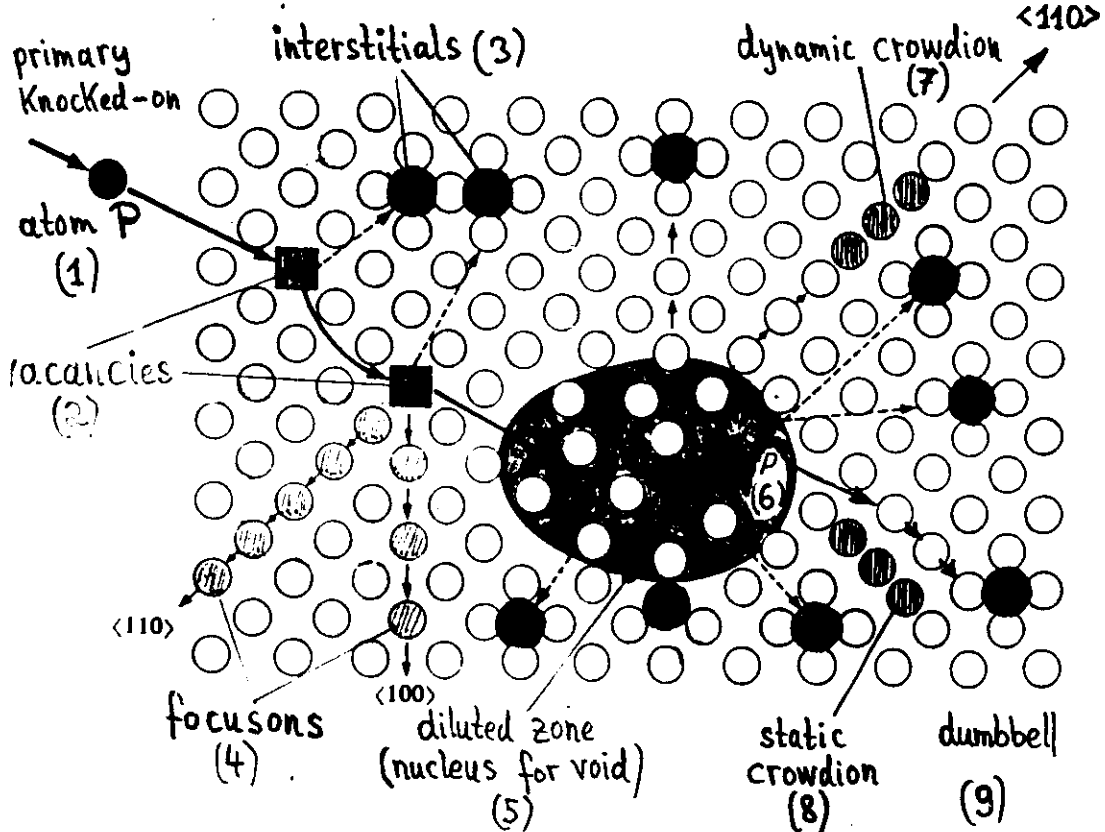
D6 Voids lattice in Nb – 1% Zr after V^+ implantation (bcc $\parallel$ bcc host lattice, 780°C, 3.1 Mev, 50 dpa)

Void lattices

- high-dose neutron or ion irradiation at about 1/3 T_m
- void lattices ≡ host lattices

Radiation Damage by Fast Neutrons

(fcc metal, (100) plane)

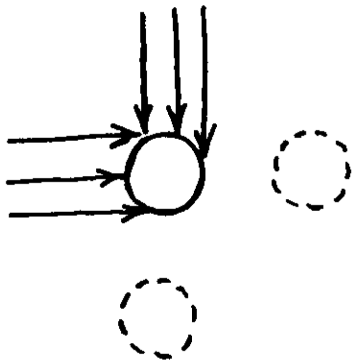


1) "Ballistic" athermal transport: dynamical crowdions

2) Thermally activated diffusion of point defects:

one-interstitial model	two-interstitial model
vacancies (3d)	vacancies (3d)
dumbbells (3d)	stable dumbbells (3d)
	metastable crowdions (1d)

Void-Lattice Formation by Mutual Protection of Voids against Dynamic Crowdions (Foreman)



Arguments against this mechanism

Void hyperlattices in Al (Horsewell & Singh)

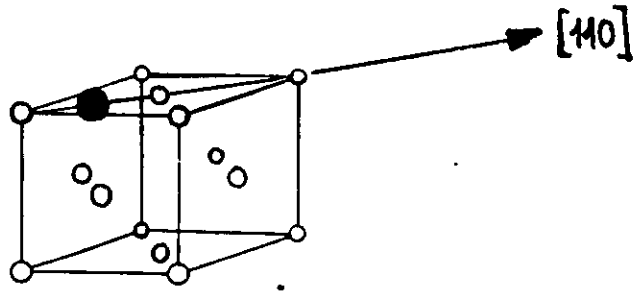
(required range of dynamic crowdions ≃ 2A = 400 ... 500 nm)

Metal	packing density	dynamic crowdions	void lattices	static crowdions
Au	● ● ●	+++	—	—
Nb	● ● ●	++	+	+
Al	• • •	+	+ +	++

Two-Interstitial Model

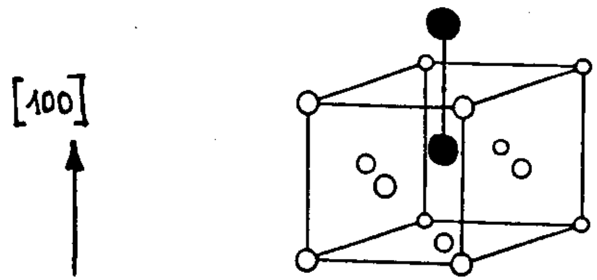
(fcc metals)

(static) crowdion (1d)

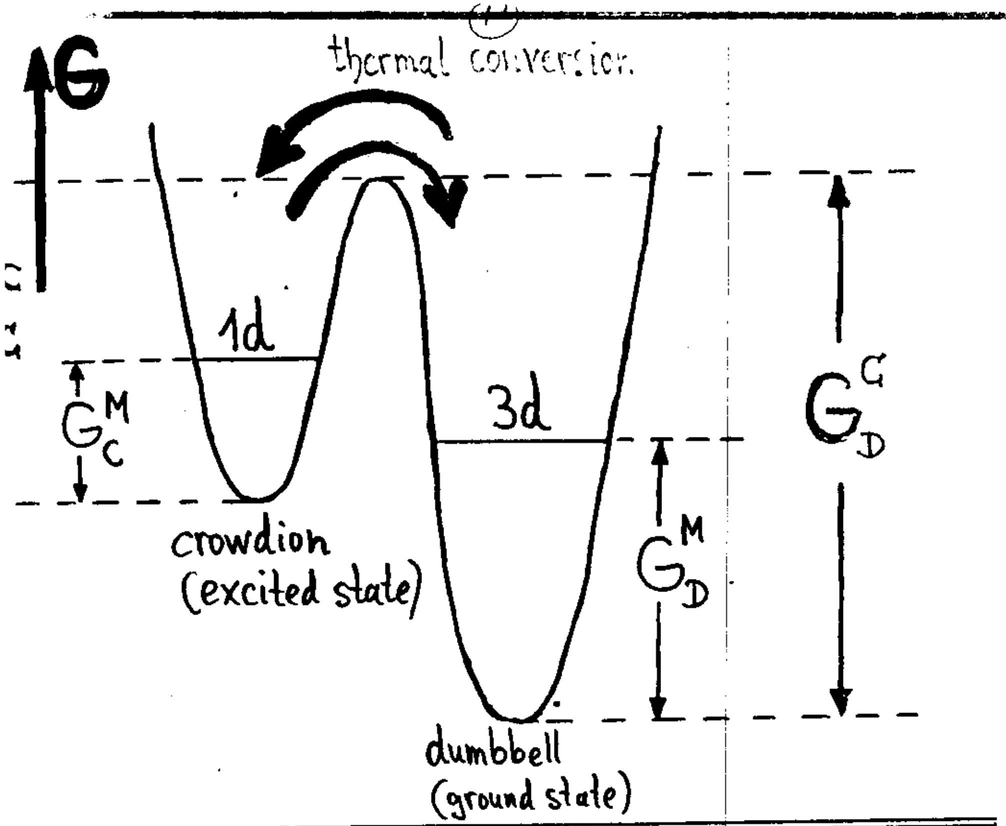


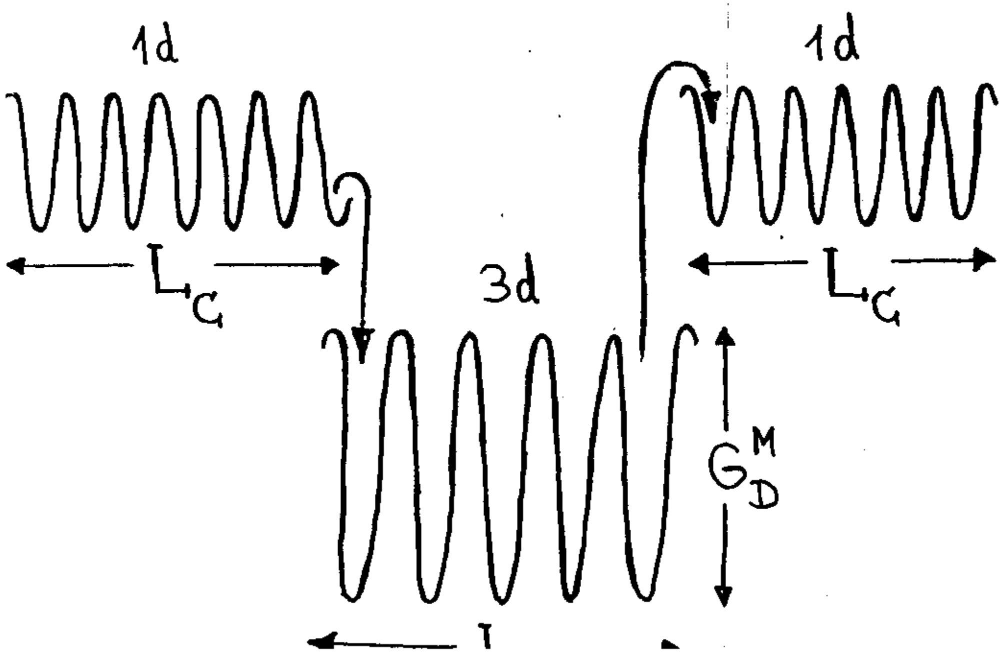
= metastable excited interstitial state

dumbbell (3d)



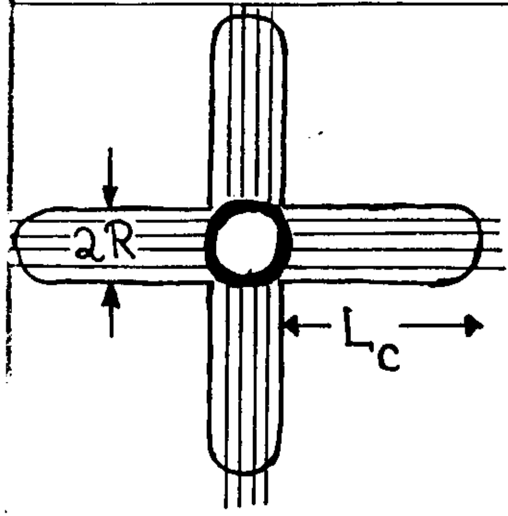
= ground state of interstitial



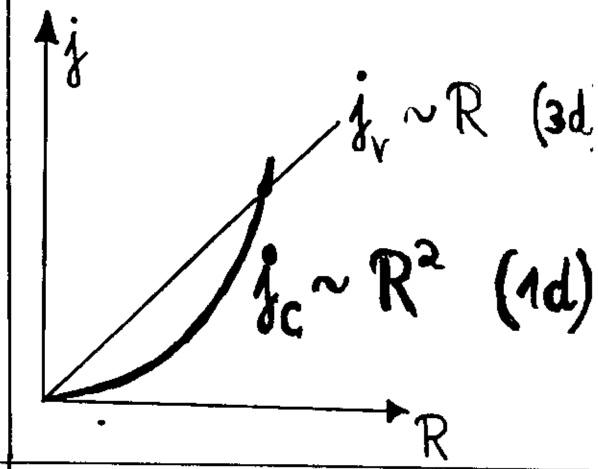


Theory of Void-Lattice Formation

(Woo & Frank 1985, Hähner 1989)



capturing cylinders for crowdions adjacent to voids



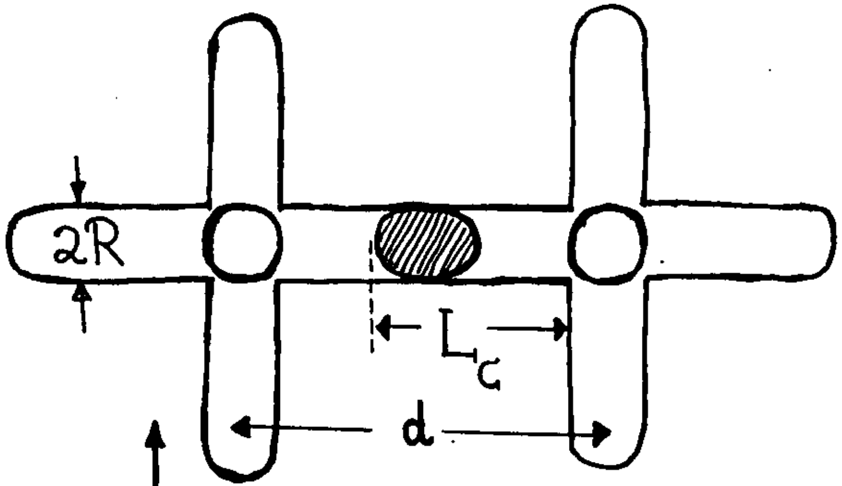
symmetry breaking by anisotropic diffusion of crowdions

$$j_V^{net} = j_V - j_D - j_C$$

- voids grow until a final size is reached
- disordered arrangement of voids is conserved
- only true for low void densities (at which capturing cylinders of neighbouring voids do not overlap)

void density — a control parameter!

High void density (capturing cylinders do overlap)



$$\dot{j}_V^{net} = \dot{j}_V - \dot{j}_D - \dot{j}_C$$

- overlapping leads to enhanced growth rate
- isolated voids shrink away

➡ **Void-Lattice Formation by Darwinian Selection!**

- void lattices and host lattices possess the same structure and orientation
- quantitative result :
  undamped mode : $d \simeq 2R + 0.7\, L_C$

Chronology of Void-Lattice Formation

1) Establishing of quasi-steady concentrations of vacancies, dumbbells, and crowdins
2) Nucleation of statistically arranged voids at the diluted zones in displacement cascades
3) Growth of voids in disordered arrangement

↓

- high void density → (see 4)
- low void density → standstill of void growth in disordered arrangement

4) Void-Lattice Formation by Darwinian Selection

↓

Standstill of growth of lattice voids

Theory of Stacking-Fault-Tetrahedron Lattices

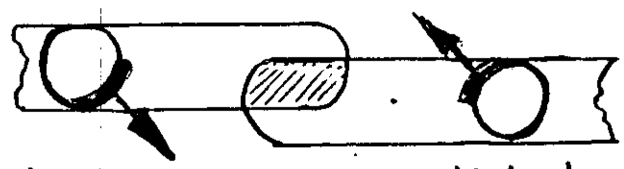
(Zaiser 1991)

- "Low" temperatures, high defect densities, suppression of thermal diffusion, but extensive radiation-induced diffusion
- 1-dimensional transport of matter by dynamic crowdions (symmetry breaking)
- Defocusing of dynamic crowdions in inter= stitial-rich regions
  → periodic accumulation of interstitials (distance $\simeq L_{G,\,dynamic}$)
- Periodic accumulations of vacancies in the intermediate regions
  → "CsCl" lattice
- Collapse of vacancy-rich regions to stacking-fault tetrahedra arranged in a primitive-cubic lattice (|| fcc host lattice)

Void Lattices Versus Stacking-Fault-Tetrahedron Lattices

> What is the crucial difference between the mechanisms of formation?

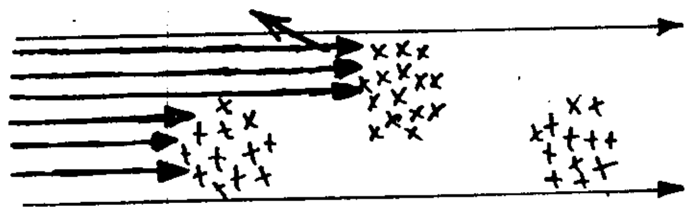
Void lattices — selective distruction:



→ alignment in close-packed directions

→ void lattice ≡ host lattice

Stacking-fault-tetrahedron lattice — selective construction:



→ disalignment from close-packed directions

→ Stacking-fault-tetrahedron lattice ≢ host lattice