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INTERNATIONAL ATOMIC ENERGY AGENCY
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Research Workshop on Condensed Matter Physics
30 June - 22 August 1997
MINIWORKSHOP ON
QUANTUM MONTE CARLO SIMULATIONS OF LIQUIDS AND SOLIDS
30 JUNE - 11 JULY 1997
and
CONFERENCE ON
QUANTUM SOLIDS AND POLARIZED SYSTEMS
3 - 5 JULY 1997

"Learning about melting with solid helium"

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These are preliminary lecture notes, intended only for distribution to participants.

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LEARNING ABOUT MELTING WITH SOLID HELIUM

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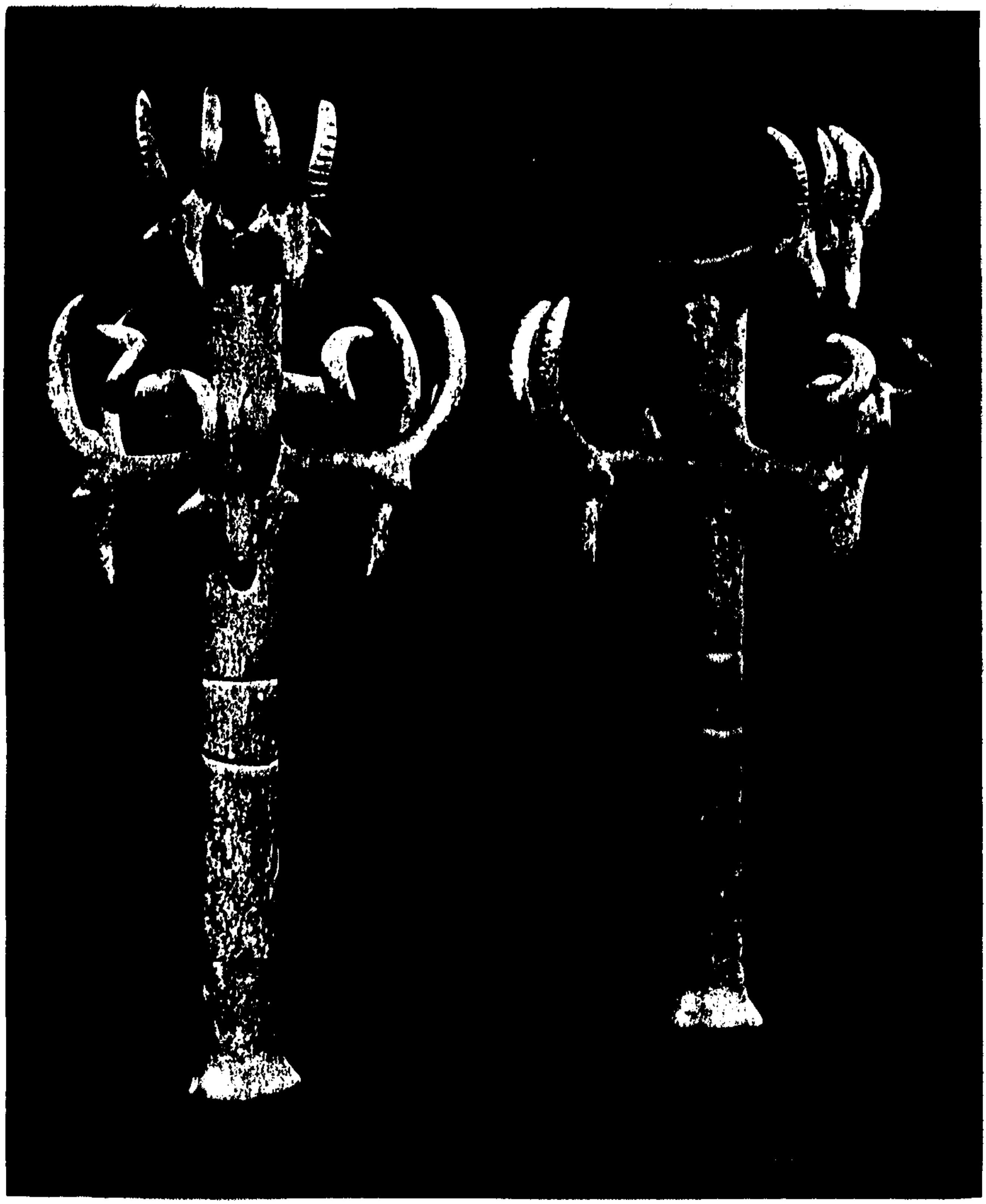
TECHNION PHYSICS DEPARTMENT

MELTING - A WELL KNOWN PHASE TRANSITION

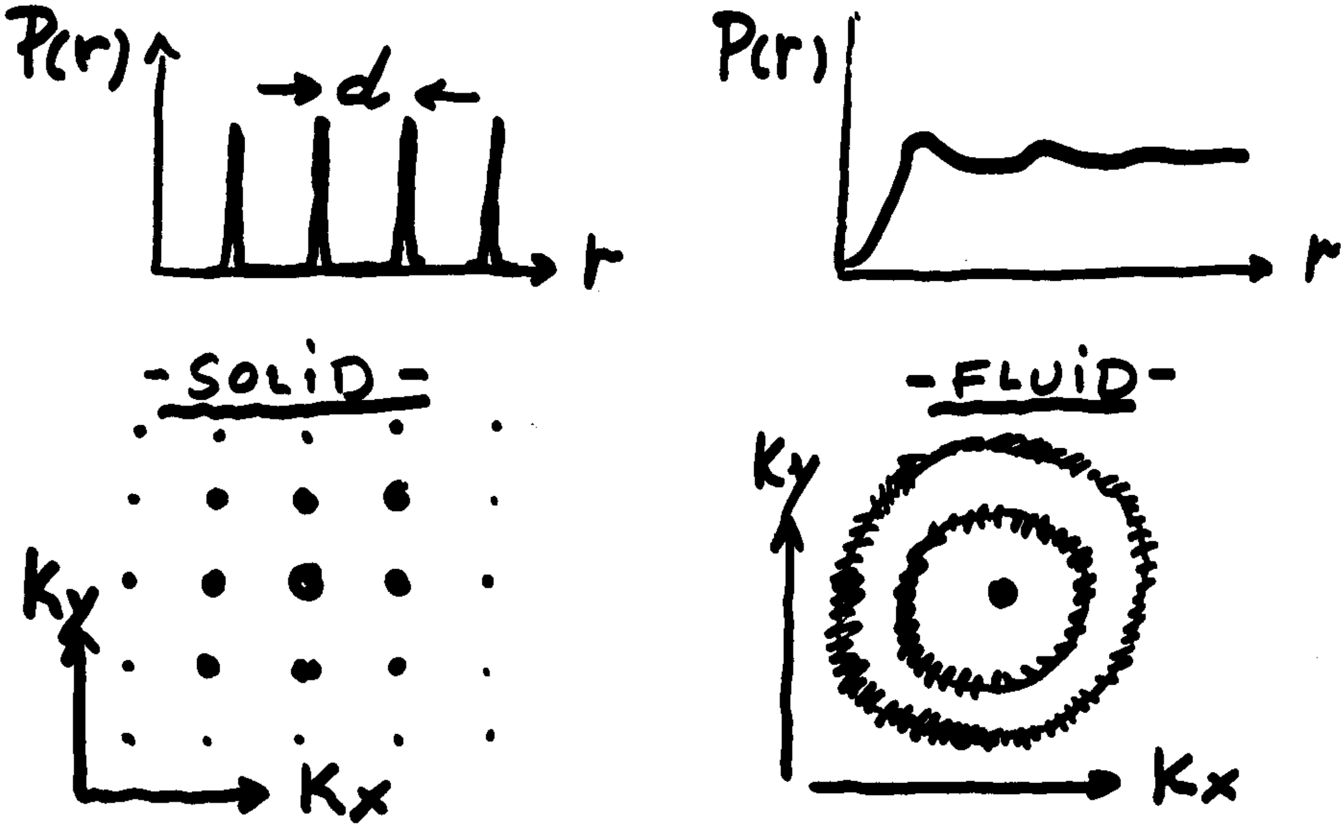


57 COPPER , 3400 B.C.

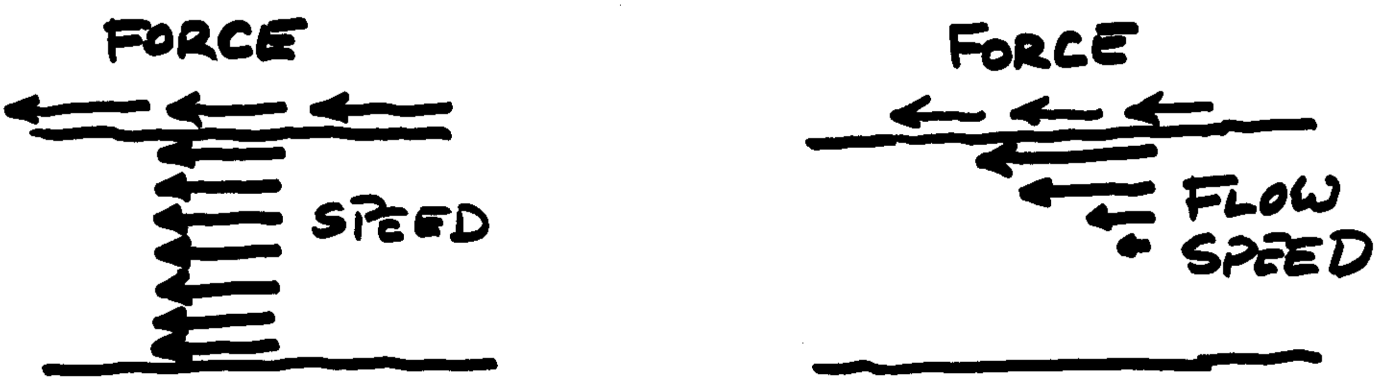
JUDEAN DESERT.

WHAT DOES ONE MEAN BY "MELTING"

a) LOSS OF LONG RANGE ORDER.



b) LOSS OF RESISTANCE TO SHEAR (10^{15})



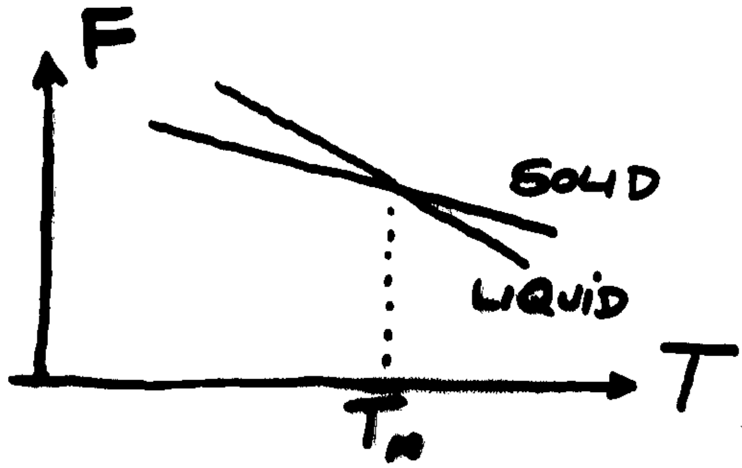
SOLID

FLUID

$F/A = \eta \frac{dv}{dy}$

THEORIES OF 3-D MELTING.

THERMODYNAMICS:



HARD!

SINGLE PHASE THEORIES:

LOOK FOR STRUCTURAL DEFECTS OR EXCITATIONS WHICH WILL DISINTEGRATE THE SOLID:

LINDEMANN (1910) - PHONONS

BORN (1939) - SHEAR INSTABILITY (also phonons)

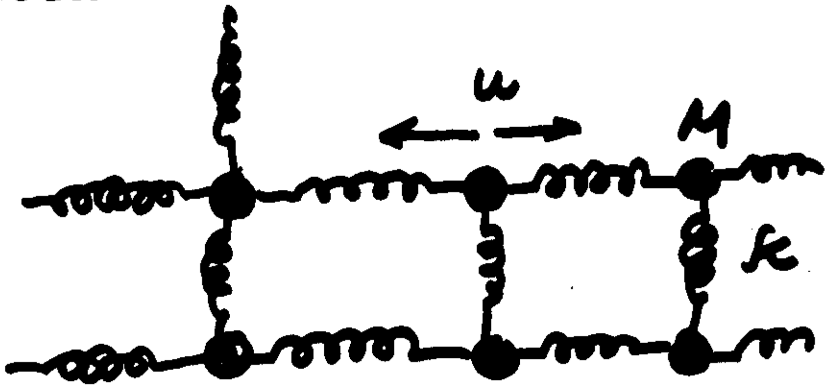
FRENKEL (1955) - VACANCIES

MIZUSHIMA (1960) - DISLOCATIONS

GRANATO (1992) - INTERSTITIALS

⋮

LINDEMANN'S MODEL



ASSUME : FOR $u > u_c$, SOLID BREAKS UP

USE :

$$\frac{3}{2} k u_c^2 = \frac{3}{2} k_B T_M$$

$$k_B \theta_D = \hbar \omega_D = 2\pi \sqrt{k/M}$$

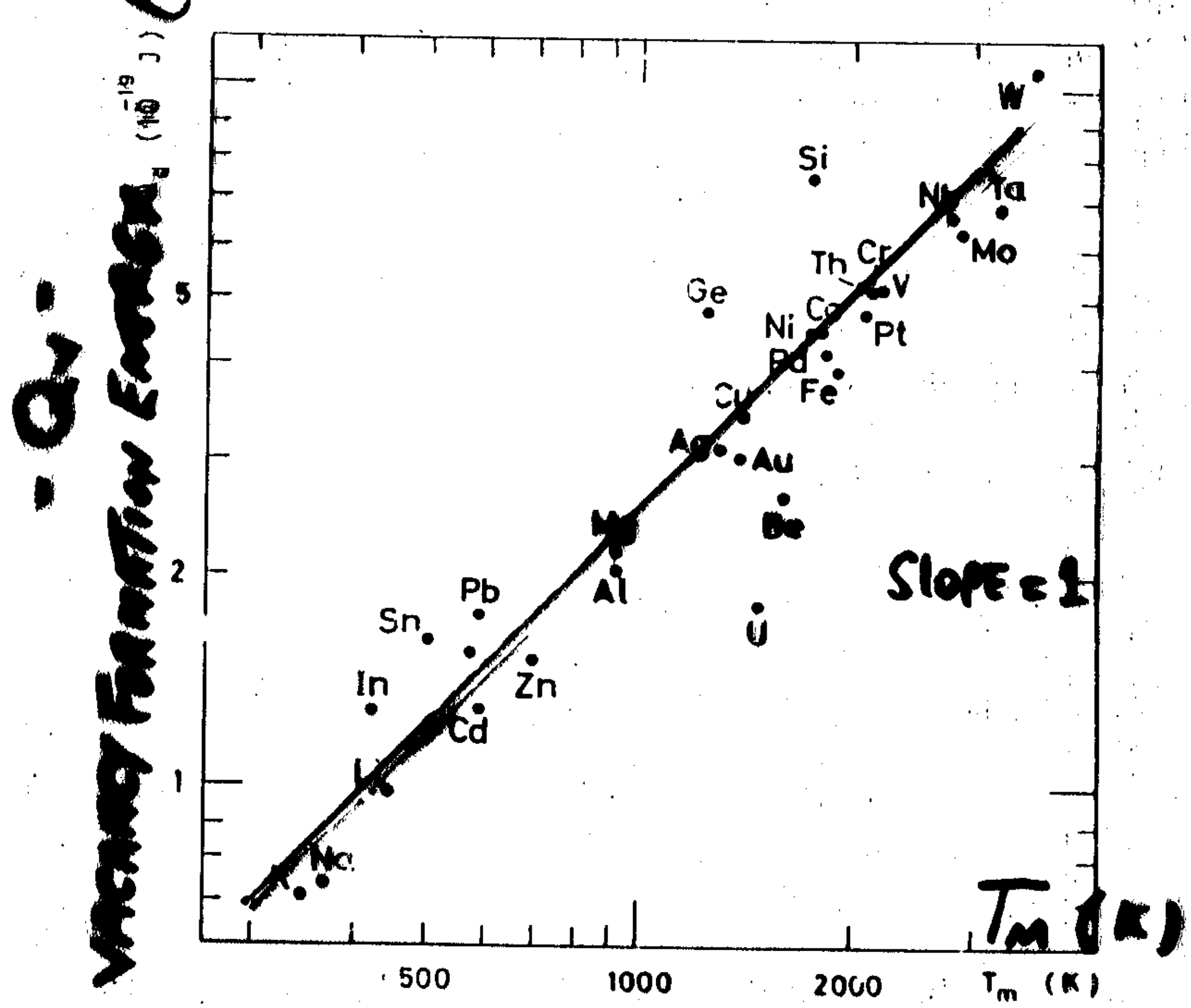
GET :

$$\boxed{\text{CONST} = \sqrt{\frac{k_B T_M}{M \theta_D^2 V^{2/3}}}}$$

WORKS FOR SOLID HELIUM! (Dugdale & Domb)

DOES NOT WORK FOR OTHER MATERIALS.

MELTING - 3D - VACANCIES



$$T_M = \text{const.} \times Q_v$$

Van Liempt (1935) - EMPIRICAL RULE

FRENKEL (1955) - THEORY

NUMBER AT $T_M \sim 10^{-3}$ (SMALL)

$$N_v = e^{-Q_v/kT}$$

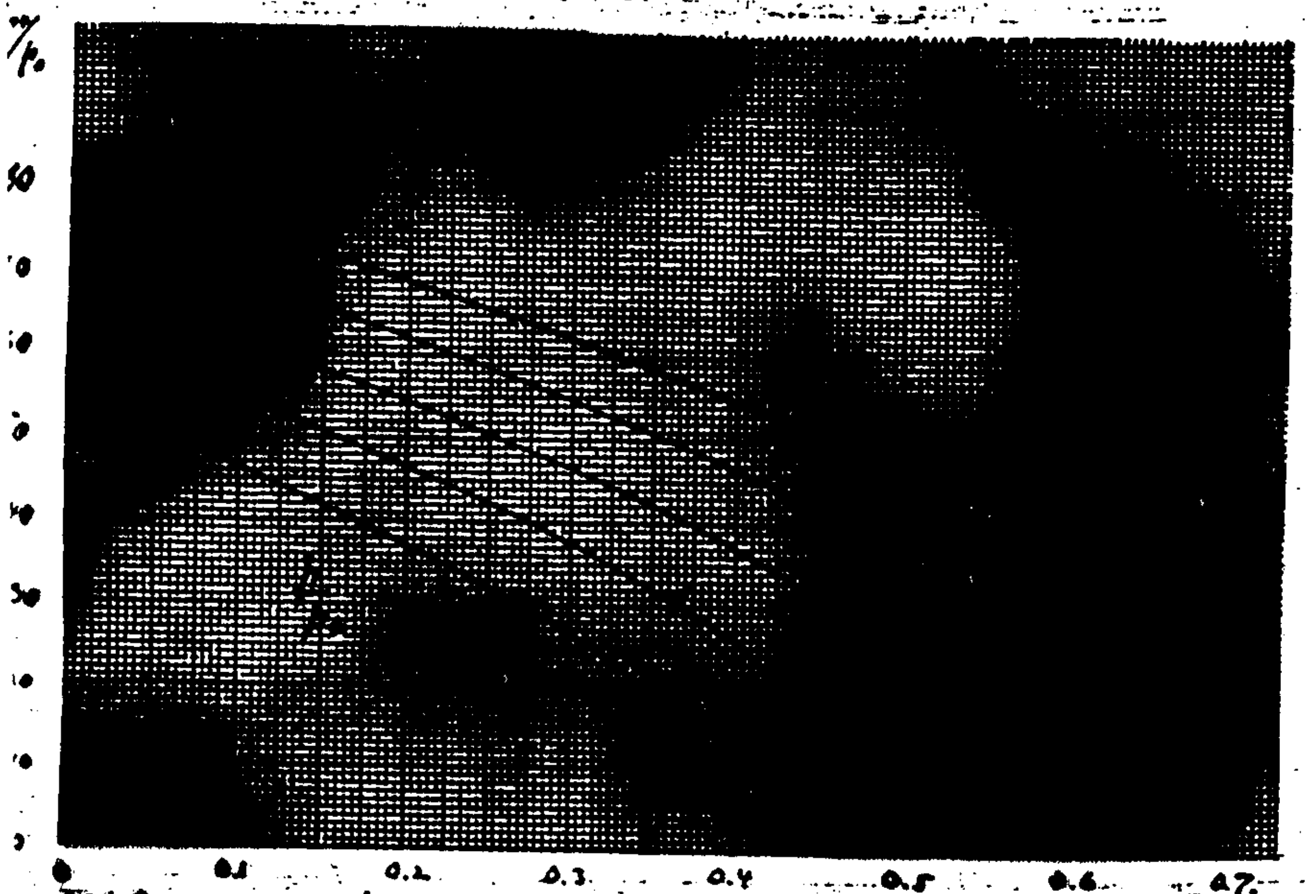
Thermodynamics of Crystals and Melting

MAX BORN
Tait Professor of Natural Philosophy, University of Edinburgh, Edinburgh, Scotland

(Received May 25, 1939)

The Helmholtz free energy, A, of a rigid body is a function of temperature, and of the six homogeneous strain components. If the crystal is to be rigid, three inequalities must be satisfied for the derivatives of A with respect to the six strain components, for a regular (cubic) lattice. This enables one to limit the pressure-temperature range for which the crystal is stable. The violation of the condition $c_{44}>0$, that the crystal resist shearing, is interpreted as leading to melting. From a knowledge of the forces between the molecules the phase integral, and therefore the free energy, may be calculated as a function of T, V, and the six strain components. The numerical calculations are carried out for a body-centered cubic lattice. The product of all the frequencies is calculated directly, so that the assumption that the Debye equation for the frequency distribution holds, is not necessary. The melting curve, pressure against temperature, is then determined.

$C_{44} \leq 0 \Rightarrow$ INSTABILITY!

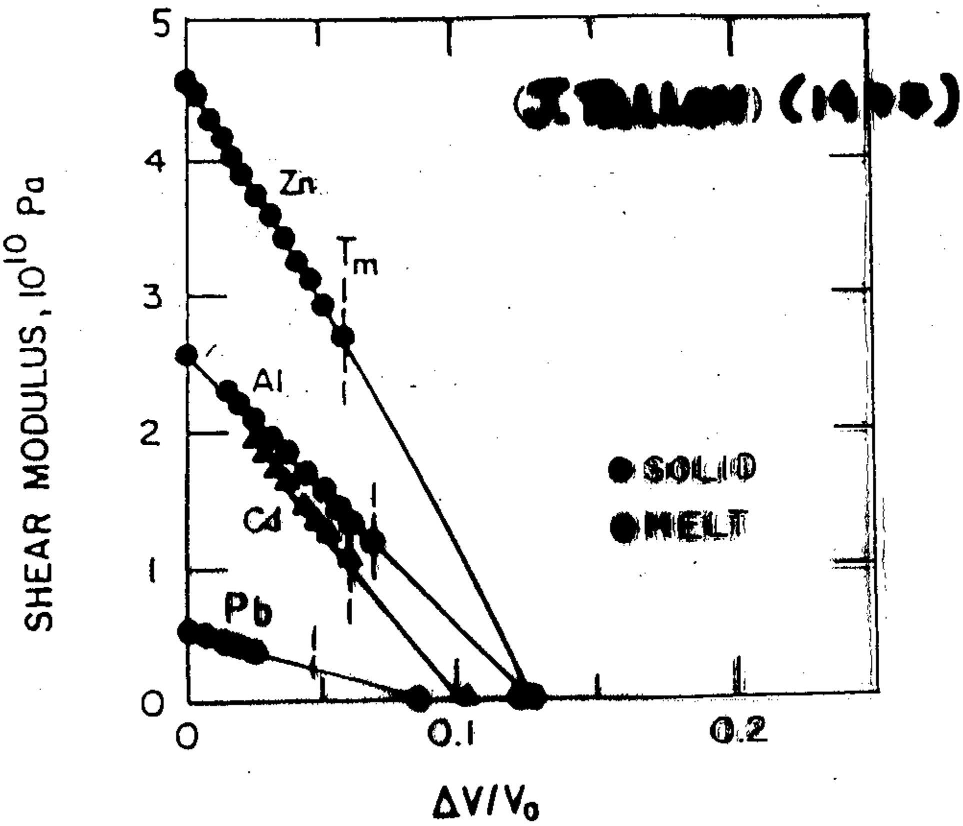


T/Θ Elasticity constant c_{44}, for $\varepsilon = 9/16$:

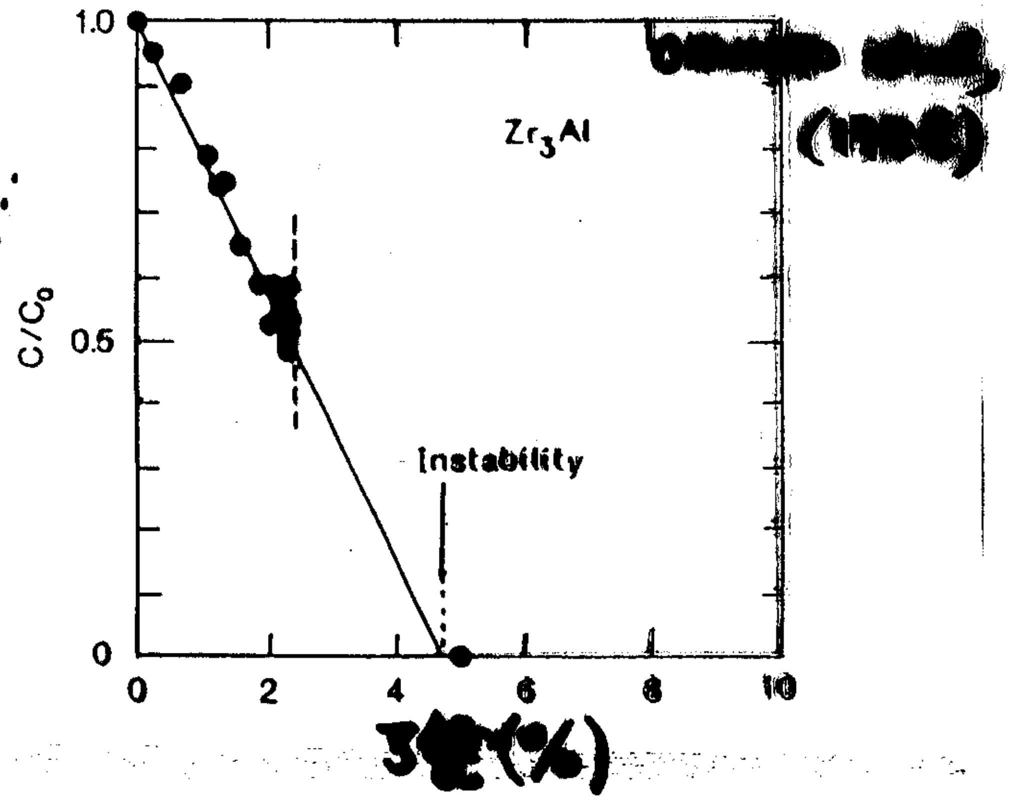
FIG. 6

C_{44} INSTABILITY: RESULT OF THERMAL EXPANSION

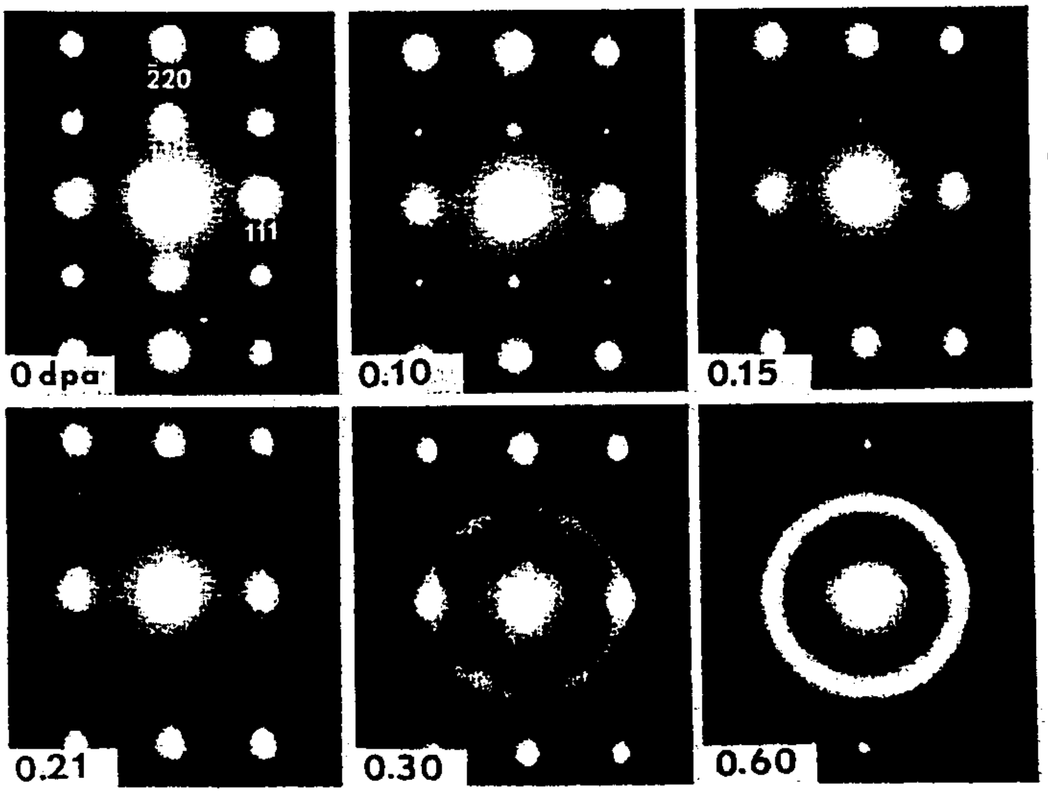
MELTING:



AMORPHIZATION:



AMORPHIZATION – LOSS OF LONG RANGE ORDER

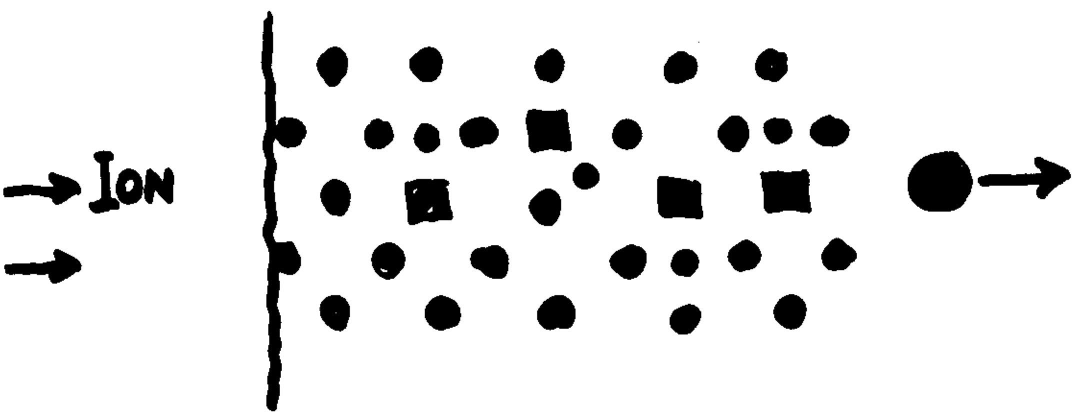


OKAMOTO et al, (1988)

d.P.A.

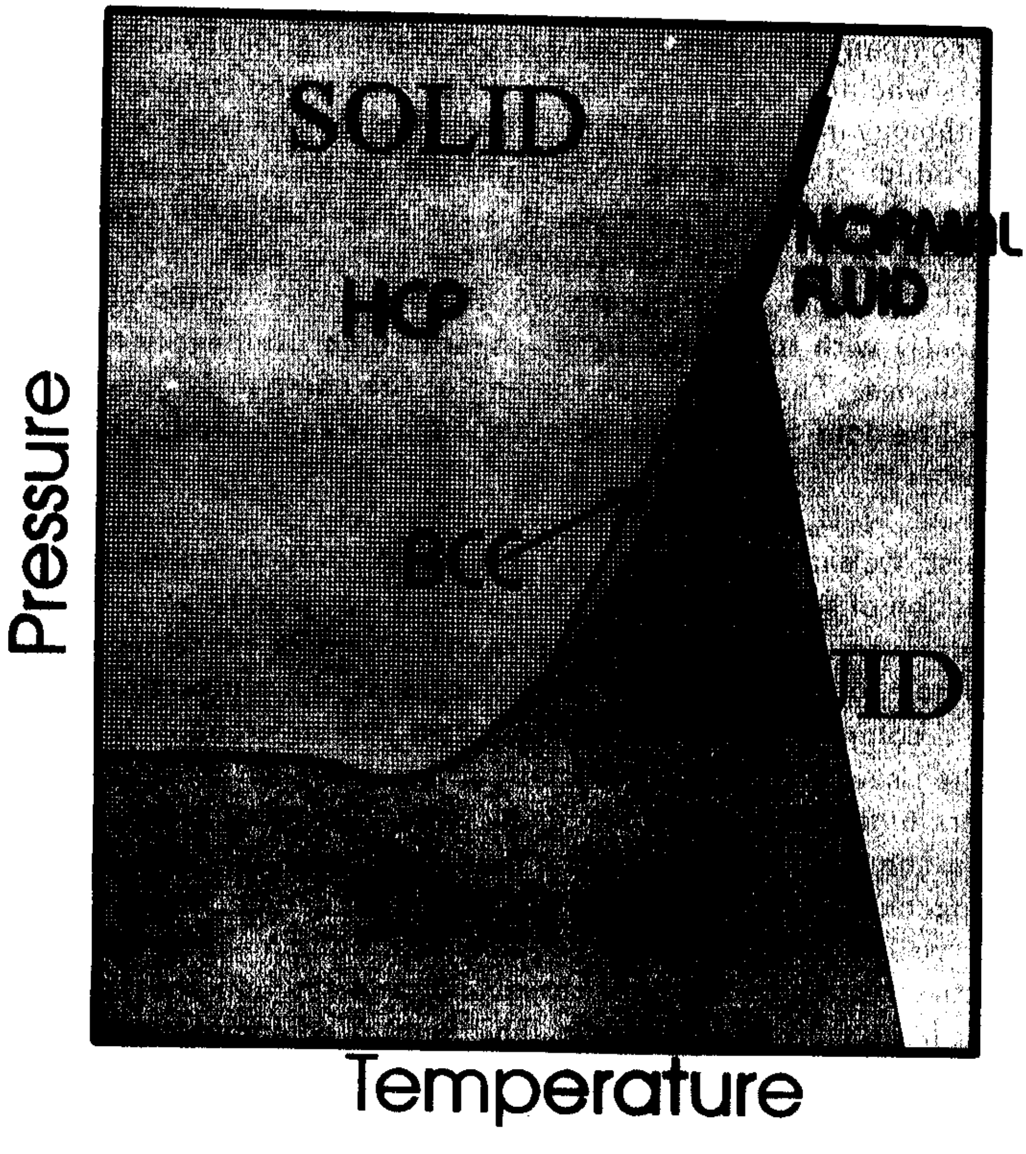
Zr_3Al

Fig. 3. Sequence of [112] zone-axis diffraction patterns of Zr_3Al showing the disappearance of superlattice reflections, and the formation of diffuse rings during *in situ* irradiation at room temperature with 1.0 MeV Kr^+; doses are in d.p.a.



DAMAGE: VACANCY – INTERSTITIAL PAIRS

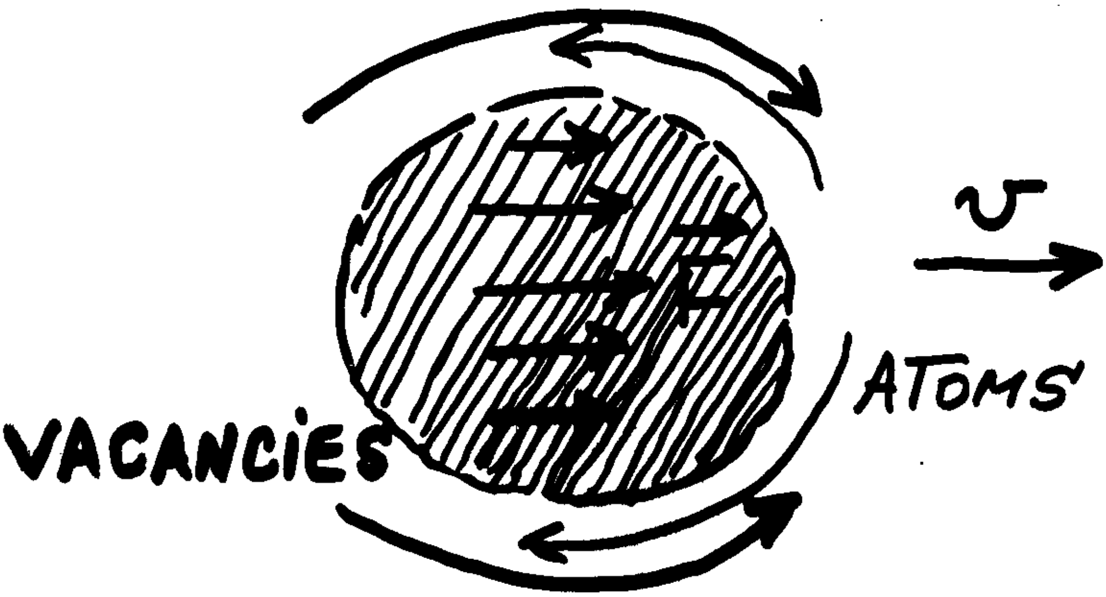
^{4}He PHASE Diagram



Experiments were carried on the melting curve, along the purple line.

MOVING WIRE EXPERIMENT

(PURE ^4He , bcc , MELTING CURVE)

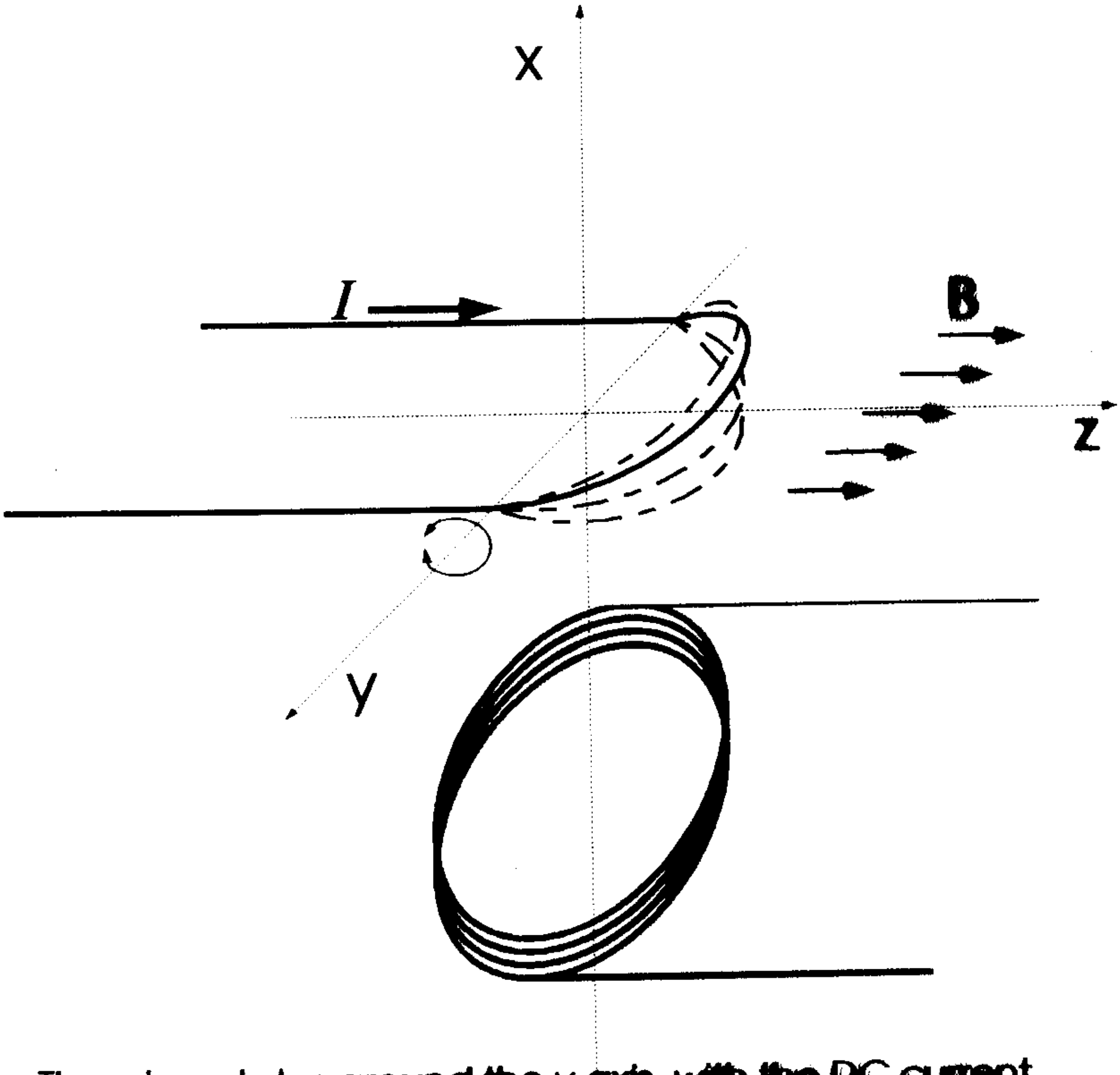


DIFFUSION COEFFICIENT:

$$D \cong \frac{kT v \rho R}{F}$$

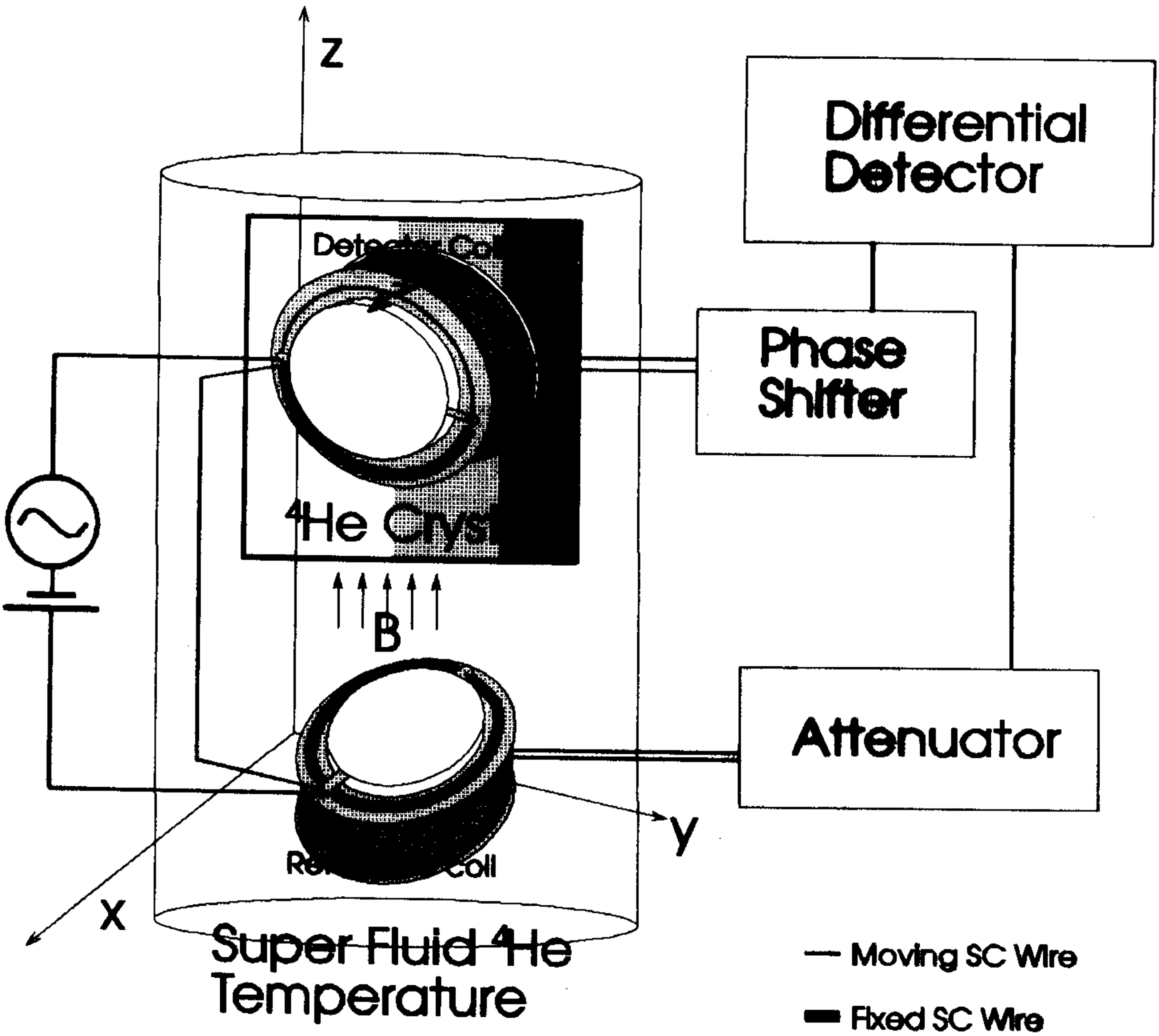
PREVIOUS EXPTS.	TECHNIQUE
DYUMIN, et al..	A. GUENAULT
SUZUKI	⋮
ELBAUM, et al.,	

Measurememt principle



The wire rotates around the y axis. with the DC current.
The induced voltage in the coil changes with the wire position.

Experimental setup



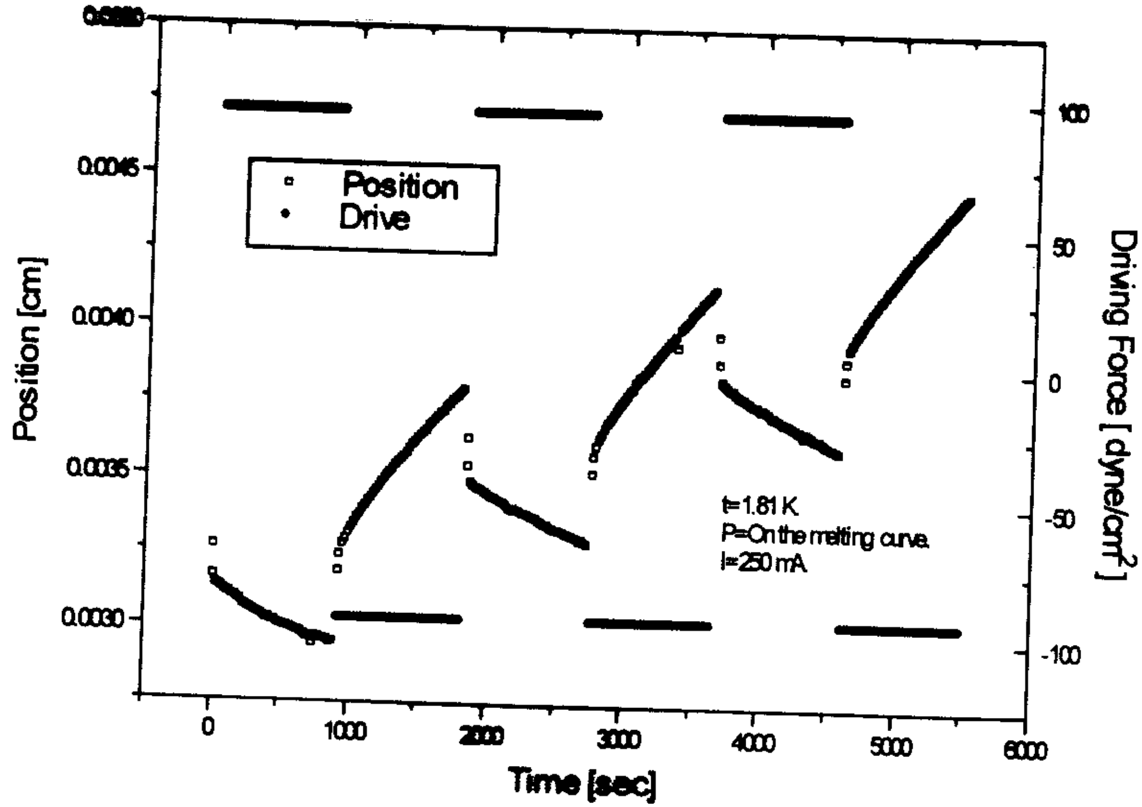
A DC, and a low amplitude, 7 Khz, AC current flows throgh the superconducting wire (— & ▬).

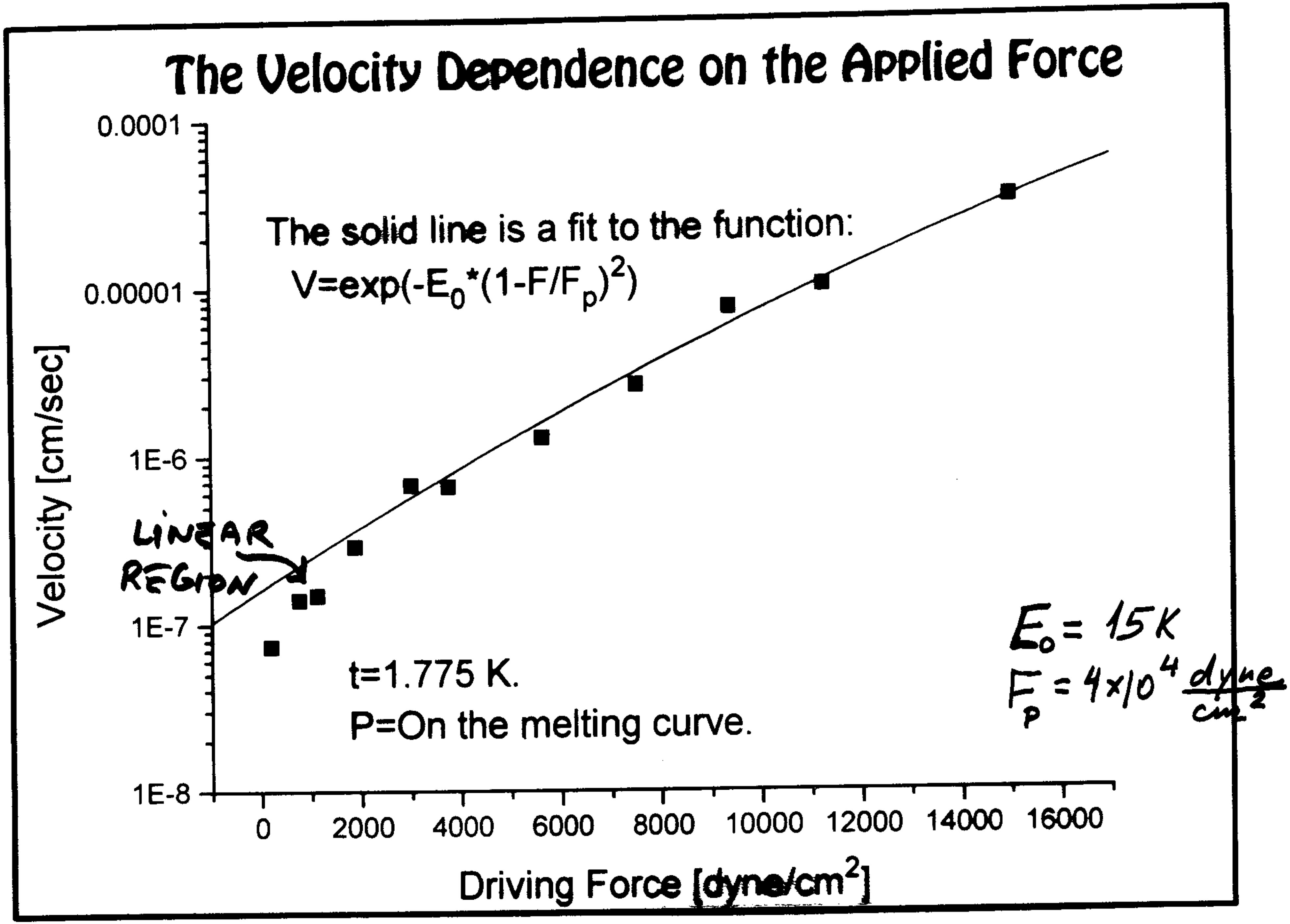
The Lorentz force, on the wire (—), drive it throgh the He crystal (▭).

The wire position is found from the induced voltage difference between the coils.

Typical Measurement Results

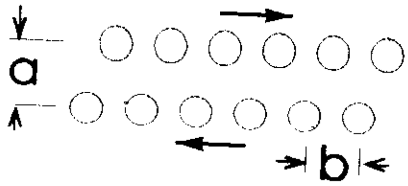
A DC current was applied to the superconducting wire. The wire, submerged in the helium crystal, moved. The difference in the induced voltage, between the cell and the reference coils is plotted here, calibrated to distance units. The current direction was periodically changed so that the drift could be subtracted.




The Velocity Dependence on the Applied Force
The solid line is a fit to the function:
V=exp(-E0*(1-F/Fp)^2)
Velocity [cm/sec]
0.0001
0.00001
1E-6
1E-7
1E-8
0
2000
4000
6000
8000
10000
12000
14000
16000
Driving Force [dyne/cm^2]
LINEAR REGION
t=1.775 K.
P=On the melting curve.
E0 = 15 K
Fp = 4x10^4 dyne/cm^2

How can one move through the crystal?

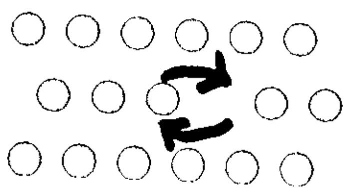
Glide of one plane other the over??



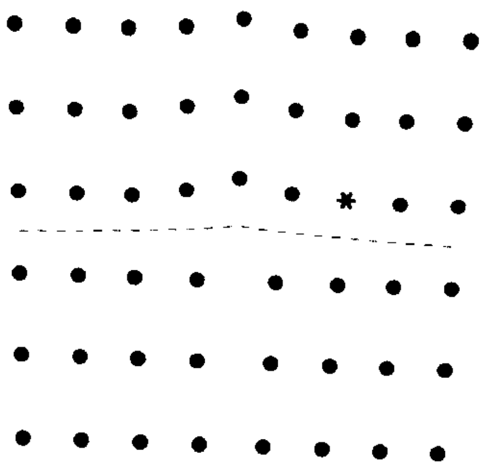
NO! - The stress needed is too high.

$$\sigma_m = \frac{b}{a}\frac{\mu}{2\pi}.$$

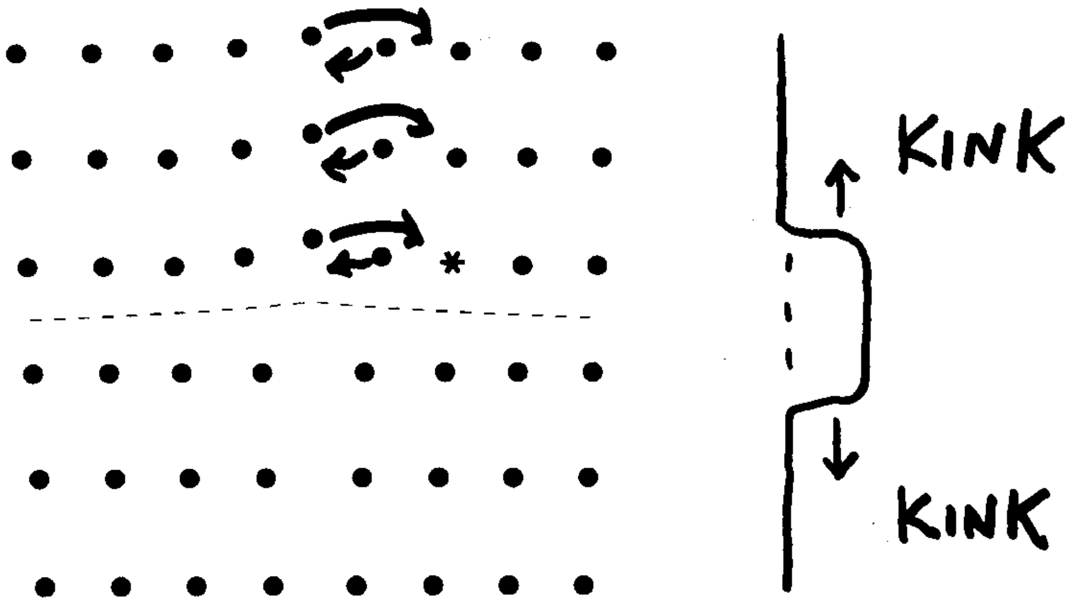
Instead of the whole plane, move a single atom-*Vacancies* mechanism. This leads to strain rate linear in the stress.



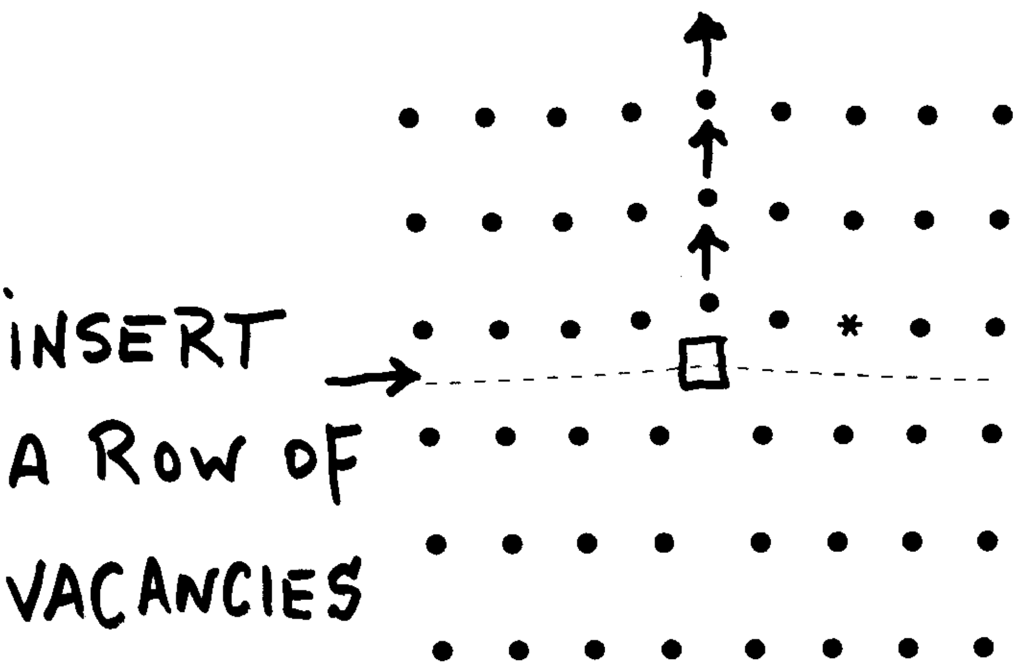
Or move a row of atoms- *Dislocation* mechanism.



GLIDE – V is EXPONENTIAL in FORCE



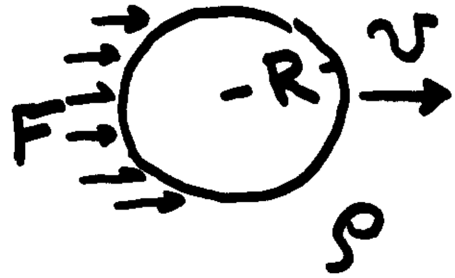
CLIMB – V is SOME POWER LAW OF FORCE



BOTH MECHANISMS HAVE AN ACTIVATION ENER

LINEAR DEPENDENCE (VACANCIES)

$$\vec{v} = \frac{D}{\rho R kT} \vec{F}$$

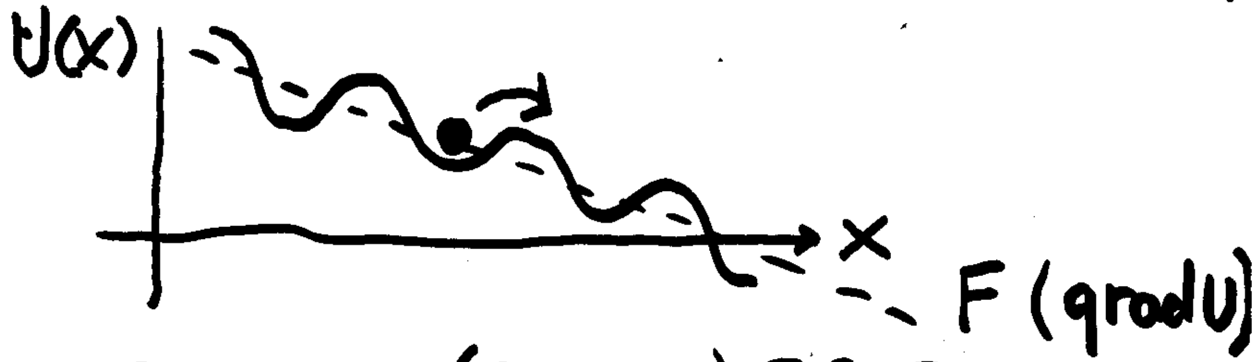


(STOKES LAW)

EXPONENTIAL DEPENDENCE (DISLOCATION GLIDE)

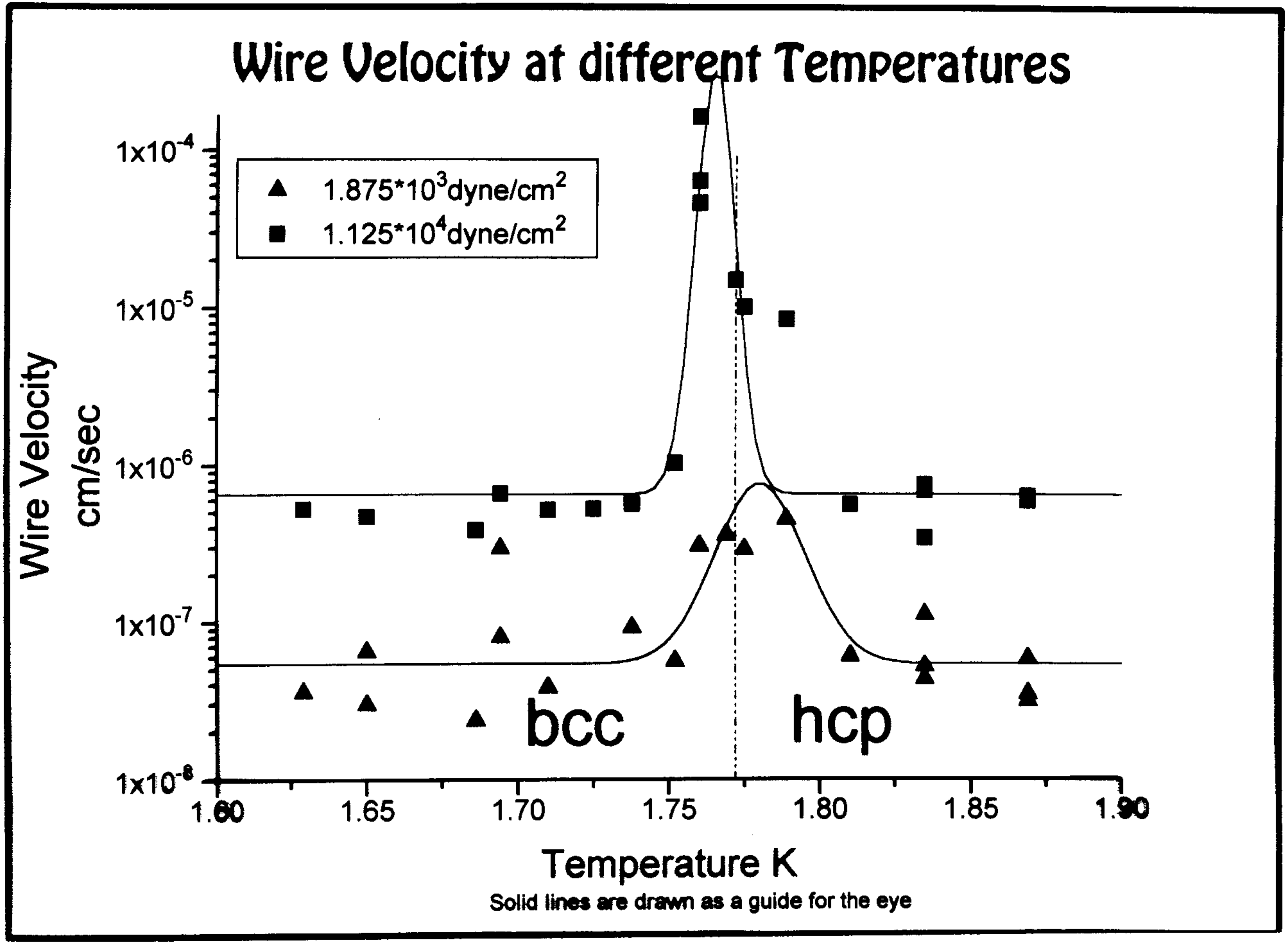
$$\vec{v} \propto \exp\left(-U_0\left(1 - F/F_p\right)^2 / kT\right)$$

(SORT OF ANDERSON-KIM CREEP MODEL)



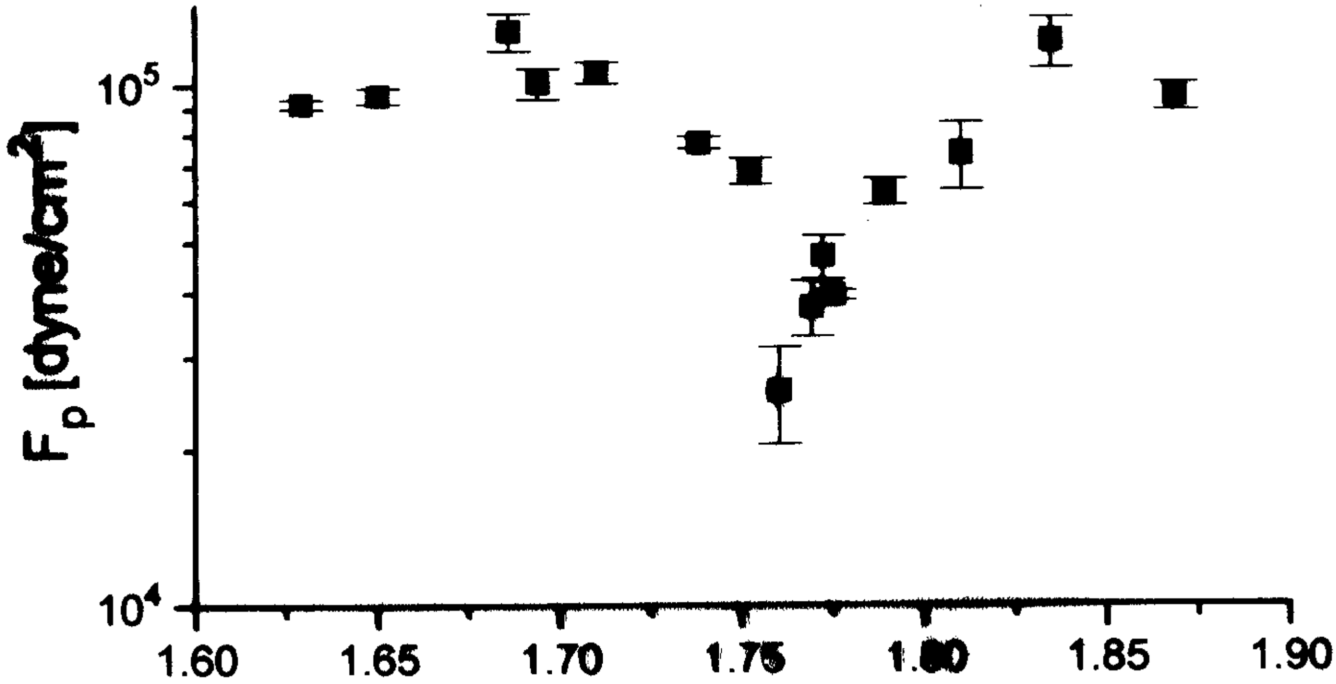
F_p – PEIERLS (PINNING) FORCE

U_0 – ACTIVATION ENERGY OF A PAIR OF KINKS

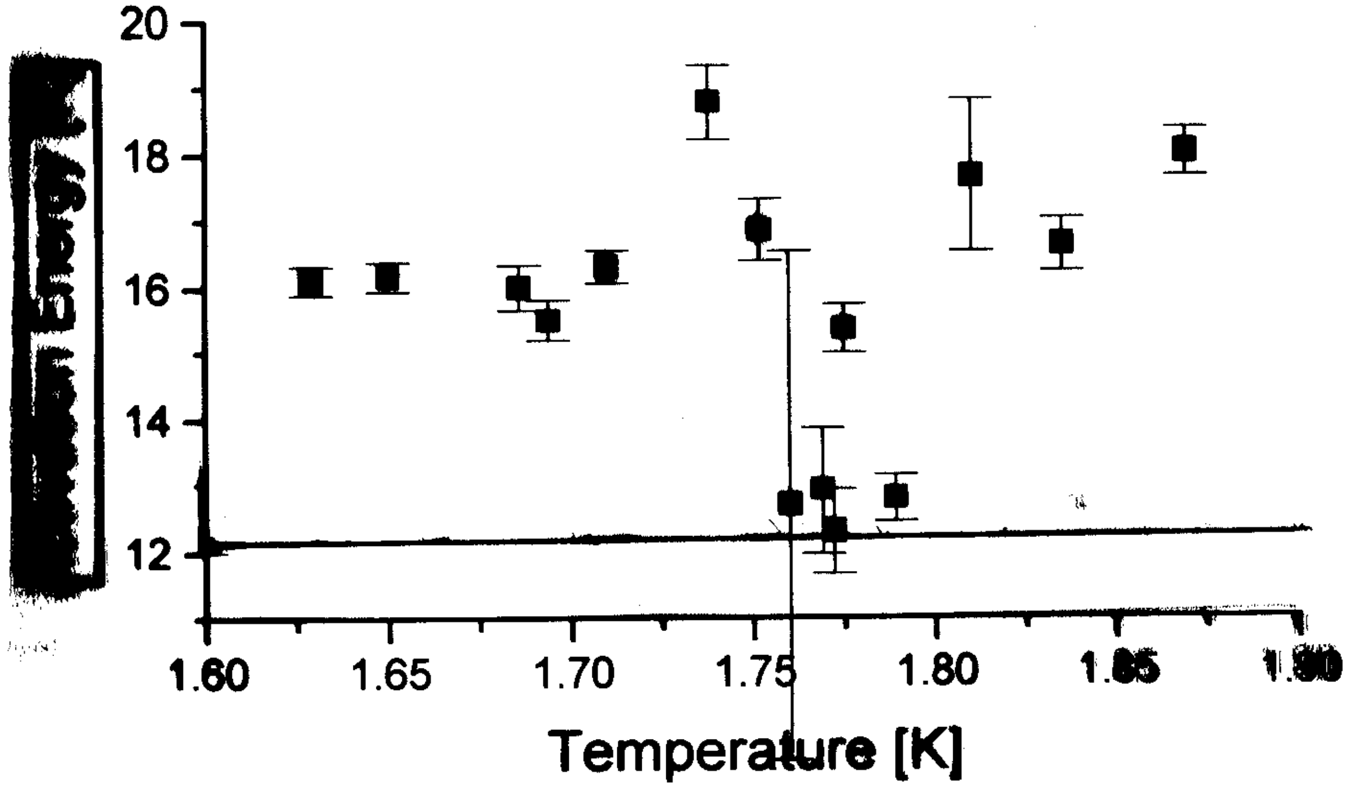


Wire Velocity at different Temperatures
1.875*10^3 dyne/cm^2
1.125*10^4 dyne/cm^2
Wire Velocity cm/sec
1x10^-4
1x10^-5
1x10^-6
1x10^-7
1x10^-8
1.60
1.65
1.70
1.75
1.80
1.85
1.90
bcc
hcp
Temperature K
Solid lines are drawn as a guide for the eye

Peierls Force vs Temperature



Activation Energy vs Temperature



CONCLUSIONS

1. PLASTIC PROPERTIES CAN EXHIBIT SOMETHING RESEMBLING "CRITICAL BEHAVIOUR" NEAR 1st ORDER PHASE TRANSITION.

2. MORE THAN ONE TYPE OF DEFECT is RESPONSIBLE FOR THIS BEHAVIOUR.

3. THE NATURE OF THE NON-LINEAR BEHAVIOUR (VS. TEMPERATURE) REMAINS A PUZZLE.