



INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE



SMR/388 - 45

**SPRING COLLEGE IN MATERIALS SCIENCE
ON
'CERAMICS AND COMPOSITE MATERIALS'
(17 April - 26 May 1989)**

**POSITRON STUDIES ON DEFECTS
IN MATERIALS**

CHI WEI LUNG
Institute of Metal Research
Academia Sinica
Wenhua Road
Shenyang
People's Republic of China

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

POSITRON STUDIES on DEFECTS in MATERIALS

I. Introduction to PA

Special advantages:

Sensitive to the presence of defects.

$\sim 10^{-7}$ vacancy concentration, $\sim 10^8$ voids ($\sim 4 \text{ \AA}$)

For studies of nondilute alloys

$> 1\% \rightarrow 100\%$

For studies under wide range temperatures

Wide range of fields

metals, semiconductors, ionic solids, polymers....

mechanical engineering, materials science,

solid state physics, theoretical physics...

Not very expensive

$\sim \text{US } \$ 20,000 - 40,000.$

Disadvantages:

Use of radioactive materials.

Complicated data analysis for the lifetime technique.

Unconventional instrumentation for many metallurgy and chemistry laboratories.

Reduced sensitivity for complicated materials (trapping saturation).

Need for a standard in order to calibrate in terms of defect concentration.

Examples of successful work:

Most reliable values of single-vacancy formation enthalpy (also in refractory metals)

Detection of microvoids and void precursors produced by low-dose neutron irradiation (below TEM resolution)

Firm experimental evidence of a vacancy migration mechanism for III stage annealing in plastically deformed iron.

References

1. P. Hautojärvi, *Positrons in Solids*, Springer, Berlin, 1979.
2. W. Brandt and A. Dupasquier, *Positron Solid State Physics*, Proc. Inter. Sch. Phys. "Enrico Fermi", North-Holland Publ. Co. (1983).
3. P.C. Jain, R.M. Singru and K.P. Gopinathan, *Positron Annihilation*, Proc. ICPA-7. World Scientific, (1985).
4. C.W. Lung and N.H. March, *Cryst. Latt. Def. and Amorphous Materials*, 13 (1984) 31.
5. Proc. ICPA-8. Gent, (in press), 1988.

I. 1. Thermalization

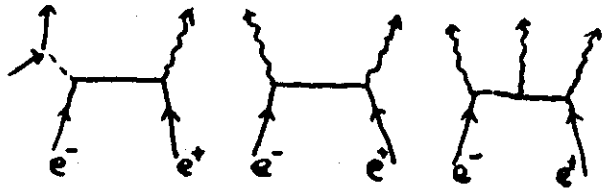
e^+ Source: ^{22}Na , ^{64}Cu , ^{57}Co , ^{68}Ge γ -ray (^{22}Na)
 (0.54 MeV) (0.65) (0.48) (1.4) (1.28 MeV)

time: $\sim 10^{-12}$ sec.

distance: 10 - 1000 μm .

energy: $kT (\sim 300^\circ\text{C}) \sim 0.025$ eV.

2. Annihilation, ($\frac{v}{c} \ll \alpha = \frac{1}{137}$)

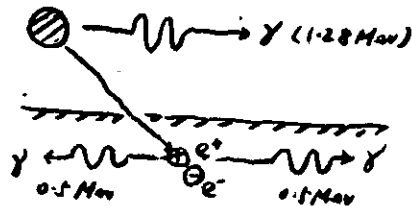


$$\sigma_{(2)}/\sigma_{(1)} \approx \alpha, \quad \sigma_{(1)}/\sigma_{(2)} \approx \alpha^2$$

$$\sigma_{(2)} = \frac{\pi r_0^2 c}{v}$$

$$\Gamma_{(2)} = \sigma_{(2)} v n_0 = \pi r_0^2 c n_0$$

$$2m_0 c^2 = 2 \times 0.511 \times 10^6 \text{ eV}$$



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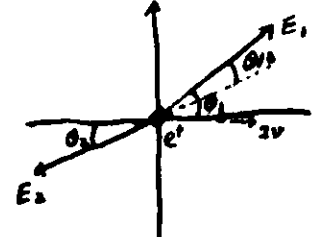
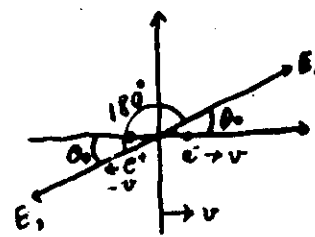
II, Lifetime $\tau = \Gamma^{-1}$

	Solid.	Liquid.	Gas.	$\tau_p < \tau_d$
τ (sec)	$\sim 10^{-10}$	$\sim 10^{-9}$	$\sim 10^{-7}$	

III. Angular correlation

e^-, e^+ static, $\vec{P}_1 + \vec{P}_2 = 0$, $\vec{C}_1 = -\vec{C}_2$; 180°

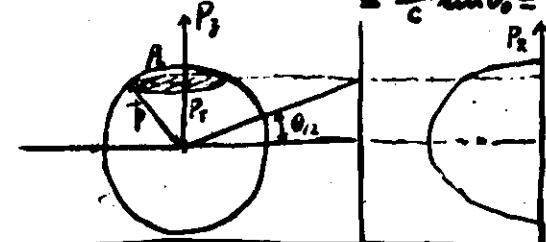
e^- motion: $\vec{P}_1 + \vec{P}_2 \neq 0$, $\vec{C}_1 \neq -\vec{C}_2$; θ_{12}



(a) axis system of center of mass, (b) laboratory axis system.

$$\sum P_z = m(v_1 + v_2) = m(v + v) = 0$$

$$\theta_{12} \approx \angle_2(\theta_1 - \theta_2) \approx \frac{\frac{1}{2} \frac{v}{c} \sin \theta_0}{1 - v^2/c^2} = \frac{1}{2} \frac{v}{c} \sin \theta_0 = \frac{P_T}{m_0 c}$$



$$N(\theta_2) = c \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dp_x dp_y \Gamma(p_x, p_y, \theta_2, m, c) = N(p_x)$$

- 5 -

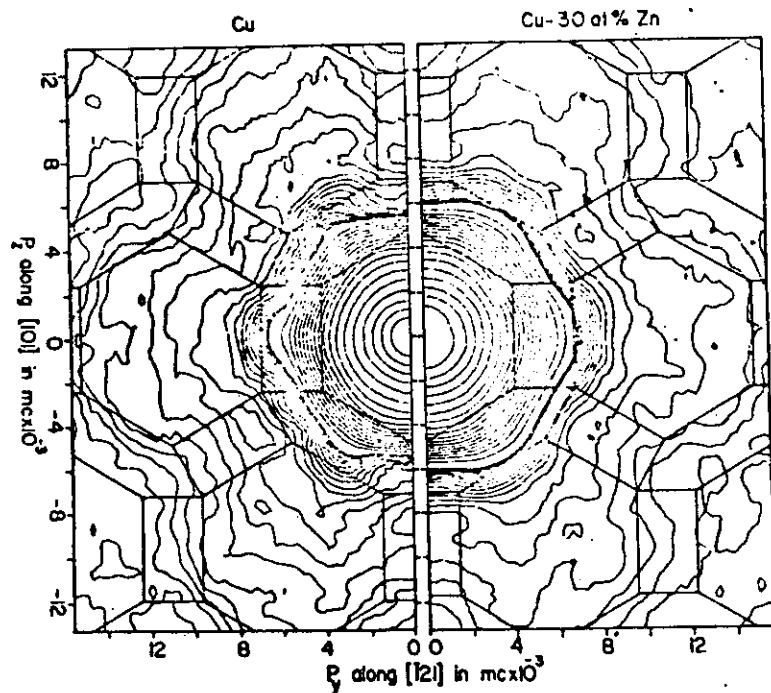


Fig. 13 The contour map of the $N(p_y p_z) - R(p_y p_z)$ surface from Cu vs Cu-30 at.% Zn, oriented with p_x along the $[111]$ direction. $R(p_y p_z)$ is a smooth rotationally symmetric surface as discussed in the text, used to exhibit the anisotropies at high momenta.

We have applied our 2D technique to the study of α -brass. Full 2D ACAR surfaces have been measured for Cu-11.6 at.% Zn [59] and Cu-30 at.% Zn, and have been compared to pure Cu [60]; we find that the momentum density is quite similar between α -brass and pure copper, except for the clear growth of the FS with alloying. We demonstrate this similarity in Fig. 13, where the contour maps of $N(p_y p_z) - R(p_y p_z)$ have been plotted for Cu and Cu-30 at.% Zn for p_x along the $[111]$ direction (corresponding to the orientation in Fig. 6). The isotropic R for Cu was the same as used in Fig. 9; the same shaped R but with a 12% reduced amplitude was used for Cu-30 at.% Zn. We note the clear growth of the FS features in the first zone. The anisotropy in higher zones is quite similar between Cu and the Cu-30 at.% Zn sample. In order to analyze qualitatively these 2D ACAR surfaces we construct from the raw $N(p_y p_z)$ a set of radial distributions $X(p, \theta)$ in the $(p_y p_z)$ plane by linear interpolation, and differentiate these distributions to obtain the breaks due to the FS. After applying resolution corrections to this analysis

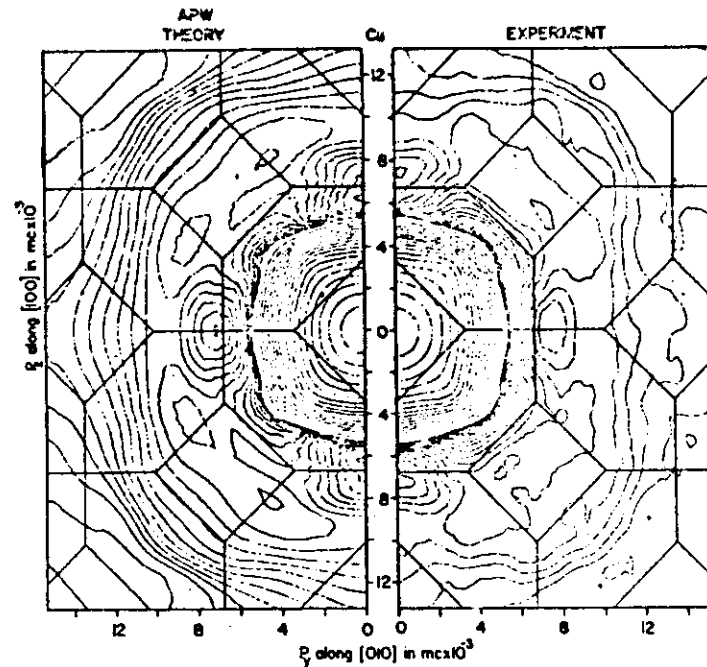
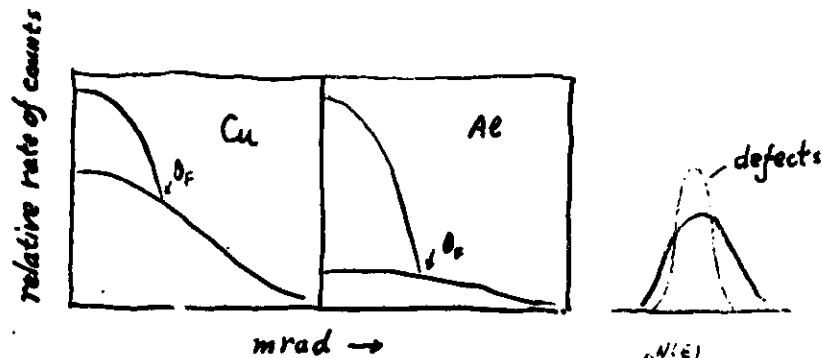


Fig. 9 Contour maps of experimental vs theoretical $N(p_y p_z) - R(p_y p_z)$ for Cu with p_x along the $[001]$ direction. $R(p_y p_z)$ is a smooth rotationally symmetric surface as discussed in the text, and is used to exhibit the anisotropies at high momenta. The steps of the contour lines are changed at around $p = 5.5$ mrad as discussed in the text.

ACAR — Angular correlation annihilation
radiation

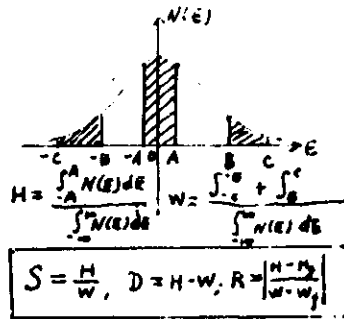


IV. Doppler broadening

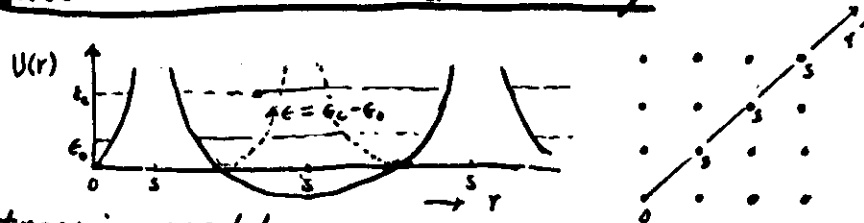
$$E_{1,1} \approx \frac{1}{2} E_T' (1 \pm \frac{v}{c} \cos \theta_0)$$

$$\approx m_0 c^2 \pm \frac{CP_L}{2} = E_0 \pm SE$$

$$P_L = 2m_0 v \cos \theta$$



V. Interaction between e^+ and vacancy



VI. trapping model

$$\frac{dn_f(t)}{dt} = -\left(\frac{1}{\tau_f} + \sum_{j=1}^m \sigma_j(t) C_j\right) n_f(t) + \sum_{j=1}^m \nu_j n_j(t)$$

$$\frac{dn_j(t)}{dt} = -\frac{n_j(t)}{\tau_j} + \sigma_j(t) C_j n_f(t) - \nu_j n_j(t)$$

$$(j = 1, 2, \dots, m)$$

Assuming: $\nu_j = 0$ (no detrapping) A. Suger
(J. Phys. F. 3 (1973) 248)

$$\sigma_j(t) = \sigma_j$$

The solution is

$$n_f(t) = n_f(0) \exp(-t/\tau_0)$$

$$\left(\frac{1}{\tau_0} = \frac{1}{\tau_f} + \sum_{j=1}^m \sigma_j C_j\right)$$

$$n_j(t) = \tau_0 \tau_j \frac{\sigma_j C_j}{\tau_0 - \tau_j} n_f(0) \exp(-t/\tau_0) +$$

$$[n_j(0) - \tau_0 \tau_j \frac{\sigma_j C_j}{\tau_0 - \tau_j} n_f(0)] \exp(-t/\tau_j)$$

$$j = 1, 2, \dots, m.$$

For spherical attractive potential wells, one obtains

$$\sigma_j(t) = \frac{4\pi r_j D}{\Omega} [1 + r_j (\pi D t)^{-1/2}] \quad \text{Waite's theory}$$

$$\text{or } \sigma_j(t) \approx \frac{4\pi r_j D}{\Omega}$$

where Ω is the atomic volume, and D the diffusion coefficient.

$$k = \left\{ \begin{matrix} \sigma \\ \mu \end{matrix} \right\} C_t \leftarrow \begin{matrix} \text{trapping rate} \\ \text{specific} \end{matrix} \text{ concentration of traps of type } j$$

$$\bar{\tau} = \frac{\int_0^\infty [n_f(t) + \sum_{j=1}^{\infty} n_j(t)] dt}{n_f(0) + \sum_{j=1}^{\infty} n_j(0)}$$

$$\bar{\tau} = \tau_f \cdot \frac{1 + \sigma \tau_{iv} C_{iv}}{1 + \sigma \tau_f C_{iv}} \quad (\text{for monovacancy})$$

$$\text{or: } \frac{\bar{\tau} - \tau_f}{\tau_f - \tau_f} = \frac{\sigma C_{iv}}{1 + C_{iv} \sigma}; \quad \boxed{\frac{\bar{\tau} - \tau_f}{\tau_f - \bar{\tau}} = \tau_f \sigma C_{iv}}$$

$$\sigma = \frac{4\pi D r_{iv}}{\Omega}$$

$$\bar{\tau} = \tau_f \cdot \frac{1 + (4\pi r_{iv} C_{iv} \tau_{iv} D / \Omega)}{1 + (4\pi r_{iv} C_{iv} \tau_f D / \Omega)}$$

$$C_{iv} = \exp(S_{iv}^f / k) \exp(-H_{iv}^f / kT)$$

$$\boxed{H_{iv}^f = kT \left[\frac{S_{iv}^f}{k} + \ln \left(\frac{4\pi D r_{iv} \tau_f}{\Omega} \right) + \ln \left(\frac{\tau_{iv} - \bar{\tau}}{\bar{\tau} - \tau_f} \right) \right]}$$

(vacancy formation energy)

VII. $\Gamma_0 = \pi r_0^2 c n_e$

$$\Gamma_0(p) = (\pi r_0^2 c) \frac{1}{(2\pi)^3} \sum_i \left| \int d\mathbf{r} \exp(-i\mathbf{p} \cdot \mathbf{r}) \psi_i(\mathbf{r}) \psi_i^*(\mathbf{r}) \right|^2$$

$\psi(\mathbf{r})$: electron wave function

$\psi_+(\mathbf{r})$: positron wave function

$r_0 = e^2 / mc^2$: the classical electron radius.

VIII. e^+ and defects $H \Psi_+(\mathbf{r}) = E_0 \Psi_+(\mathbf{r})$
pseudopotential and pseudo wave function

1. $\Psi_K(\mathbf{r}) = U(\mathbf{r} - \mathbf{R}) \varphi_K(\mathbf{r})$ (perfect crystal)

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_a(\mathbf{r}) \right] U(\mathbf{r}) = E_w U(\mathbf{r})$$

$$\left. \frac{\partial U}{\partial r} \right|_{r=R_0} = 0 \quad R_0: \text{muffin-tin radius}$$

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + w(\mathbf{r}) \right] \varphi_K(\mathbf{r}) = E_0(\mathbf{k}) \varphi_K(\mathbf{r})$$

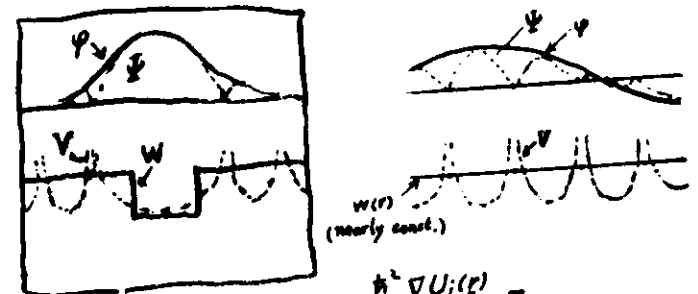
where,

$$w(\mathbf{r}) = \begin{cases} E_w + V(\mathbf{r}) + V_a(\mathbf{r} - \mathbf{R}) - \frac{\hbar^2}{m} \frac{\nabla U(\mathbf{r})}{U(\mathbf{r})} \cdot \nabla & (\text{in}) \\ V(\mathbf{r}) & (\text{between}) \end{cases} \quad (w < 0)$$

2. defect crystal

$$V(\mathbf{r}) = \sum_i V_{\text{ref}}(\mathbf{r} - \mathbf{R}_i) + \Delta V(\mathbf{r}) + V_{\text{corr}}(\mathbf{r})$$

$$V_{\text{ref}}(\mathbf{r}) = \begin{cases} V_{A_j}(\mathbf{r}), & (\text{in}) \\ 0, & (\text{outside}) \end{cases}$$



$$w(\mathbf{r}) = \Delta V(\mathbf{r}) + E_{el} + V_{\text{corr}}(\mathbf{r}) - \frac{\hbar^2}{m} \frac{\nabla U_j(\mathbf{r})}{U_j(\mathbf{r})} \cdot \nabla$$

IX. Annihilation characteristic

1-D angular correlation curve

$$I(p_2) = \int dp_1 \int dp_3 \Gamma_2(p_2)$$

isotropic: e^+e^- overlapping integral

$$I(p_2) = 2\pi \int_{p_2}^{\infty} dp \cdot \bar{p} \Gamma_0(p)$$

homogeneous electron gas: $\Gamma_0(p) = \frac{\pi r_0^3 c}{(2\pi)^3}$

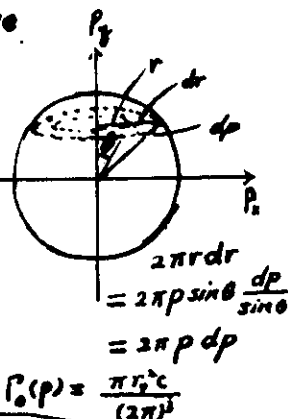
$$I(p_2) = \frac{r_0^3 c}{4\pi} (p_F^3 - p_2^3) \theta(p_F - |p_2|)$$

($|p_2| < p_F$ at, $\theta(p_2) = 1$; $|p_2| > p_F$ at, $\theta(p_2) = 0$)

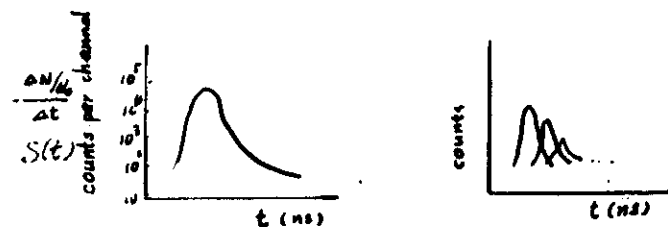
inhomogeneous electron system:

$$I(p_2) = \frac{\pi^3 c}{4\pi} \int dx |\psi(x)|^2 \lambda[n(x)]$$

where, $\lambda[n(x)] = \frac{n(x)}{4} [p_F(x)^3 - p_2^3] \theta(p_F(x)^3 - |p_2|^3)$



Vacancy studies with PA (Experiment)



The resulting experimental time spectrum $S(t)$ can be written as the sum of n components

$$S(t) = \sum_{i=1}^n I_i \Gamma_i e^{-\Gamma_i t}$$

For simplicity, we discuss the two state trapping model.

$$S(t) = I_1 \Gamma_1 e^{-\Gamma_1 t} + I_2 \Gamma_2 e^{-\Gamma_2 t}$$

$$\Gamma_1 = \lambda_f + k = \tau_f^{-1} \quad I_1 = \frac{\lambda_f - \lambda_t}{\Gamma_1 - \lambda_t}$$

$$\Gamma_2 = \lambda_t = \tau_t^{-1} \quad I_2 = \frac{k}{\Gamma_1 - \lambda_t}$$

$$(\lambda_f = \tau_f^{-1}, \lambda_t = \tau_t^{-1}, k = \sigma C_e)$$

$$\sigma C_e = I_2 \left(\frac{1}{\tau_f} - \frac{1}{\tau_t} \right)$$

$$C_e = \exp(S_H/k_B) \exp(-H_A/k_B T)$$

$$C_t \equiv C_{iv} = \exp(S_{iv}^F/k_B) \exp(-H_{iv}^F/k_B T)$$

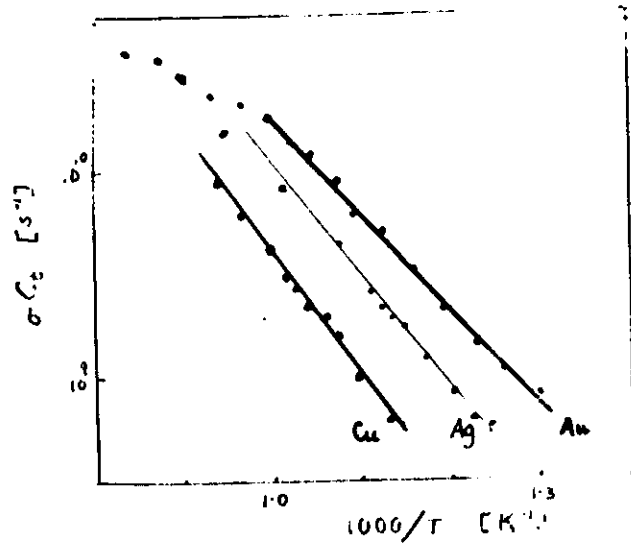


Fig. Arrhenius plots of the trapping rates σC_t with T^{-1} Proc. ICPA-7 (1985) 456
Stuck and Schaefer

Table. Vacancy formation enthalpies H_v^F by PA

Metal	H_v^F (ev)	Metal	H_v^F (ev)
Mg	0.85 ± 0.10	Ta	2.8 ± 0.60
Al	0.68 ± 0.04	Cr	2.00 ± 0.20
In	0.55 ± 0.03	Mo	3.0 ± 0.20
Cu	1.29 ± 0.07	W	4.0 ± 0.30
Ag	1.12 ± 0.07	d-Fe	1.6 ± 0.15
Au	0.89 ± 0.04	Co	1.34 ± 0.07
Zn	0.52 ± 0.07	Ni	1.78 ± 0.10
Cd	0.52 ± 0.02	Pd	1.85 ± 0.25
Pb	0.57 ± 0.06	Pt	1.32 ± 0.04
V	2.1 ± 0.20	Sn	0.50 ± 0.01
Nb	2.65 ± 0.40	U	≈ 1.0

Hydrogen release



Hydrogen charging

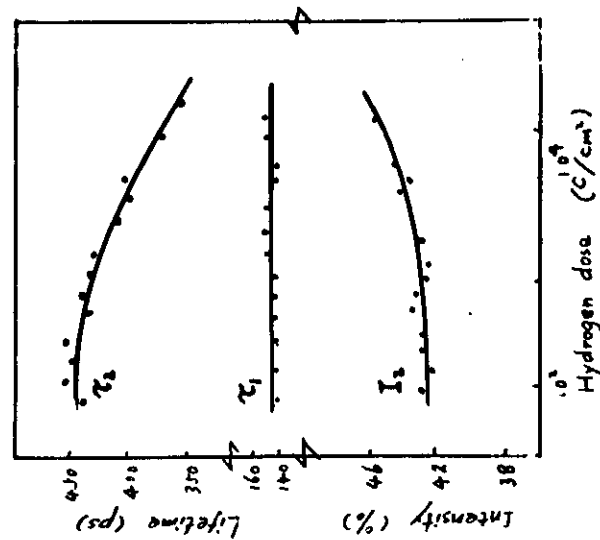
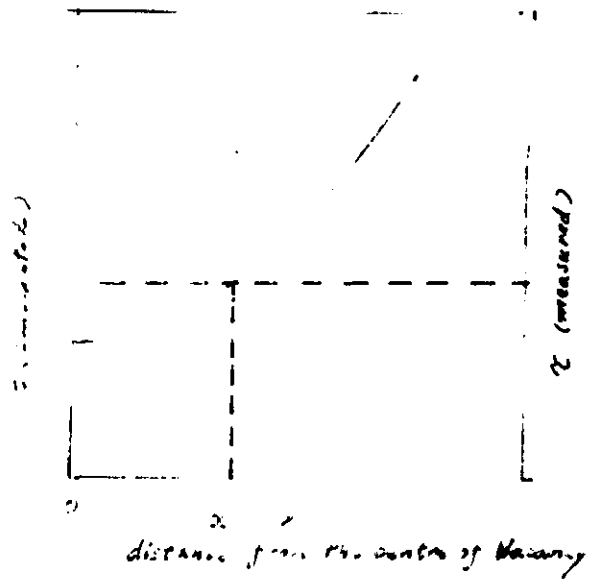


Fig. Positron lifetime parameters in Mo containing voids ($T_{prep} = 450^\circ\text{C}$) during electrolytical H injection (uncal. scale) and thermal H release.

Mo 60°C imad.
 $1.72 \times 10^{18} \text{ n/cm}^2$
annealed up to
 $450^\circ\text{C} \sim 650^\circ\text{C}$
($p < 10^{-7} \text{ po}$)
H: injected
electrolytically
in 5% H_2SO_4
solution



The position of the atom of the impurity atom-decorated vacancy can be determined by combination of theoretical calculation and PA lifetime measurements.

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DISLOCATION TRAPS

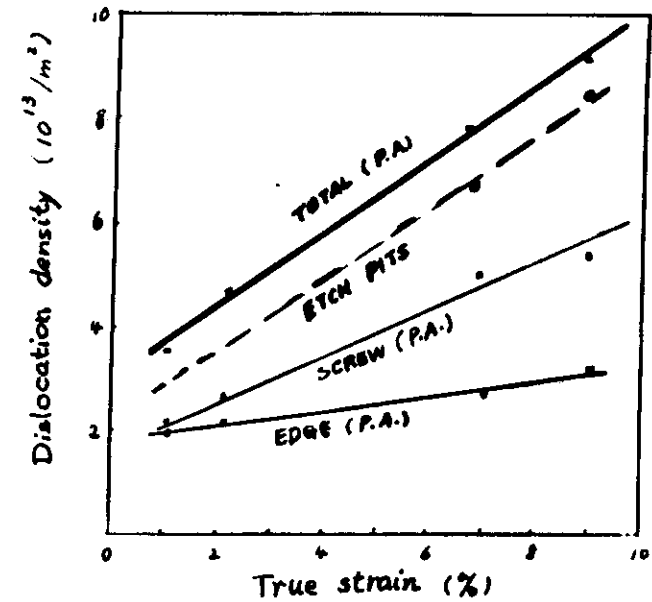


Fig. Dislocation densities measured by PA and etch pits in iron single crystals in tension at 200 K.

$$\tau_s = 142 \pm 5 \text{ ps.}$$

$$\tau_e = 165 \pm 3 \text{ ps.}$$

$$\epsilon < 10\% \quad \sigma = K_2/C_2 \approx (1-10) \times 10^8 \text{ m,}$$

$$\tau_f = 114 \text{ pscc}$$

$$\text{jog separation: } 2000 b \quad (\text{by TEM})$$

$$\text{no. of jog traps / total traps} \approx 10^{-3}$$

The unresolved (small) jogs can not be ruled out as being the sites for PA.

ICPA-7, (1984), 587

Y.M. Park et al.

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P-N dislocation core model and potential annihilation effects

位错中心 P-N 模型和正电子湮没效应

$u_x = -\frac{b}{2\pi} \tan^{-1}(\frac{x}{\xi})$
 ξ , semi width of the disl. Simple 2-D model
 ξ 是位错半宽度。 = 二维的简化模型。

$$u_y = -(b/2\pi) \tan^{-1}(\frac{y}{\xi})$$

$$u_0 = 0$$

位错中心的体积膨胀 volume expansion in the dislocation core

$$f(r) = \text{div } u$$

$$= -(b/2\pi r) \tan^{-1}(\frac{r}{\xi}) - \frac{b}{2\pi \xi} \frac{1}{1+(\frac{r}{\xi})^2}$$

$$\rho_i(r) = \rho_0 [1 + f(r)] \quad (\text{位错心离子浓度})$$

$$= \rho_0 [1 - \frac{b}{2\pi r} \tan^{-1} \frac{r}{\xi} - \frac{b}{2\pi \xi} \frac{1}{1+(\frac{r}{\xi})^2}]$$

$$\Delta\tau = \tau_d - \tau_f = 15 \text{ ps}; \quad E_b = 1.1 \text{ eV}$$

compare with binding energy due to vacancy

$$E_b^v = 2.2 \text{ eV}$$

compare with Martin and Pascher's results of disl. (1972)

$$E_b^d \approx 0.1 \text{ eV.}$$

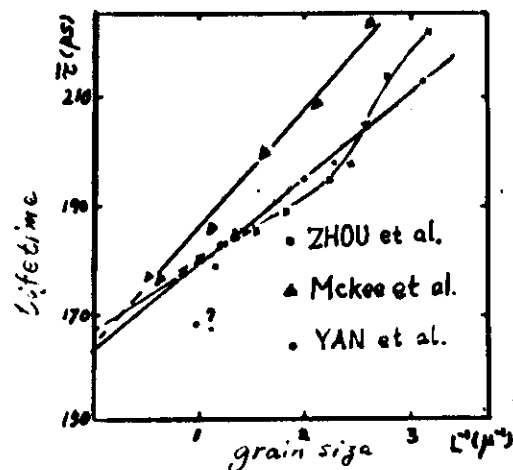
compare with Arponen et al. (1973)

$$E_b^d = 2.79 \text{ eV.}$$

Shen J. Q., LUNG C. W., Wang K. L.

Proc. ICPA-7 (1985)

phys. stat. sol. (b) 134, (1986)



Zn-22 wt.% Al

Heat treatments and measured results

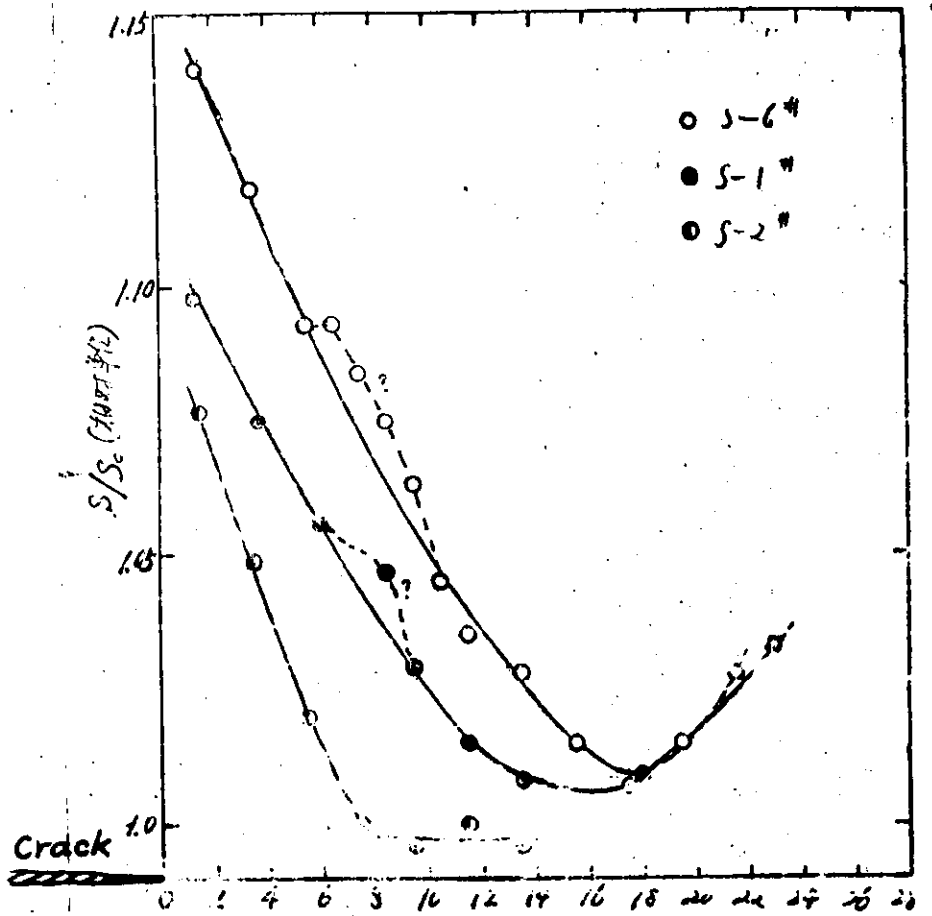
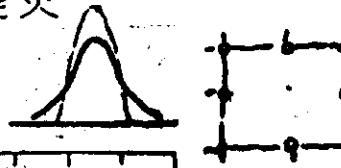
序号	Temp. Time quenching			grain size $\bar{L}$ (μm)	lifetime τ (ps)
	温度	保温时间	淬火方式		
6	350°C	0.5 hr	水盐淬	0.82	213
2	350°C	0.5 hr	水盐淬	0.39	205
	250°C		空冷		
1	350°C	0.5 hr	水盐淬	0.44	198
15	250°C	0.5 hr	炉冷	0.50	195
	350°C		水盐淬		
3	350°C	0.5 hr	水盐淬	0.76	185
	250°C		水淬		
14	250°C	0.5 hr	风冷	0.86	179
12	450°C	0.5 hr	油淬	1.02	168
16	试样初态			0.80	183

(周先京, 王淑英, 蒋惠林, 姜德, 龙翔威), 1984.

ZHOU, WANG, JIANG, JIANG, LUNG

YAN D. XIONG L. Y. & LUNG C. W. 1988.

裂缝顶端范性区的正电子湮灭



Distance 自裂端的距离 l (mm) $\rightarrow$

Positron annihilation in the plastic zone at a crack tip

in «Positron Annihilation», (1982) 469.

1981.5.

North-Holland Publ. (Jiang, Xiong, Lung et al.)

- 1, Dislocations and vacancies were mixed,
- 2 can not see DF2
3. can measure the plastic zone size*

* Xiao Jimei et al. Scripta Met. 1, 22.

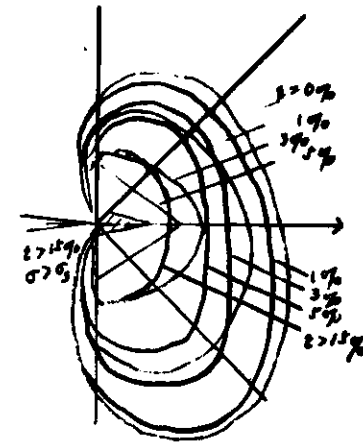


Fig. The H effects on the plastic zone of cracked 40MnNb steel measured by PA.

Tien Z. et al. Scripta Met., 16 (1982), 1383

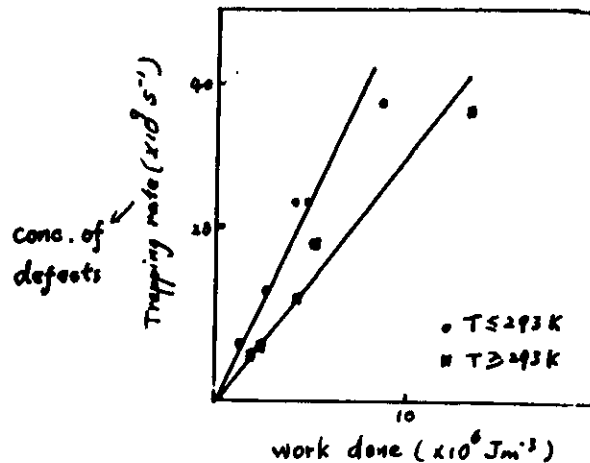
Fatigue:

- L. Diaz, R. Pareja et al. Proc. ICPA-7 (1985) 579.
 L. Diaz, R. Pareja et al. Phil. Mag. 51, 6 (1985) 461.
 S. Y. Wang et al. Proc. ICPA-7 (1985) 467.

Wang et al: (Ni polycrystalline)

1. multi-exponential fitting method, (3)
2. τ_1 : e^+ free lifetime.
3. τ_{21}, τ_{22} 209-255 $\Rightarrow$ 350 ps — $\log N$ ($N: 10 \rightarrow 10^6$)
vacancy clusters
4. τ_{1A}, τ_{1B} saturation value ~ 168 ps
dislocation loop/vacancy
5. $\tau_3 = \tau_{3A} = \tau_{3B}$ due to specimen surface.

Diaz et al.



Nanocrystalline iron

(H.E. Schaefer and R. Würschum, 1986)
 (Preprint)

Small crystallite sizes: 5-10 nm (0.005-0.01 μm)

1. volume fraction of interfacial structure
 20-50% (8-10 nm)
2. τ_1 is similar to the lifetime $\tau_{1V} = 175$ ps observed as at monovacancies in bulk iron.
3. τ_1 persist up to temperature $T = 320^\circ C$
 (not recover below this temperature)
4. τ_2 is attributed to positron trapping at microvoids at the intersection of several crystalline interfaces. (τ_2 also persists up to temperature $T = 320^\circ C$)

positronium in molecular materials (Wallace, 1960).

$$V_e > E > V_i - 6.8 \text{ eV} \quad (\text{Ore Gap})$$

V_i : Ionization potential of a molecule of the medium

V_e : the lowest excitation potential.

6.8 eV: the binding energy of the ps atom.

Ps in ionic crystals.



$$V_i > E > (V_i + Q_p) - (B.E. + Q_{ps})$$

V_i : energy required to promote an electron to the unoccupied state of lowest energy.

Q_p : energy required to remove a thermalized positron from the system.

Q_{ps} : that for the ps atom.

Let $Q_e = V_i - V_e$ (the electron affinity of the crystal).

The criterion for the existence of the Ore gap:

$$Q_e + Q_p < Q_{ps} + B.E.$$

The complexity of positron state in ionic materials.

1. Thermalization of e^+ may not be completed in some materials.
2. Formation of ps atom
 - moderate more slowly (~ 300 ps).
 - ratio of 3γ to 2γ annihilation for ps will be larger
3. Lifetime spectra are more complex than in metals. the cause of the complexity is not clear. (≈ 2 states) pure bulk effect? lattice defect trapping?
4. e^+ with a preference for negative ion cells and for interstitial regions.

$$R = S^+/S^-$$

LiF 0.08

LiCl 0.05

NaCl 0.10

KCl 0.13

KI 0.18

(S^+ : overlap on cation)
(S^- : anion)

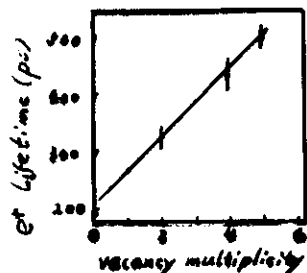
5. Positronium-like state

e^+ - negative ion bound state.

e^+ trapping at vacancies in Si

- lifetime increases linearly

- does not seem to show any saturation at 500 ps (comparing to metals)



- $\tau_0/\tau_b \sim 1.23$

(less than in metals, indicating weaker positron binding and localization at monovacancy.)

- The e^+ trapping mechanism is an open problem! trapping may depend on temperature and the charge state of a defect.

e^+ trapping at F-centres in ionic crystals

Substance	F-centre density (10^{19} cm^{-2})	$\tau(\text{ns})$	$I(\%)$	κ
NaCl	0.5	1.09 ± 0.02	4 ± 1	< 1
KCl	1	0.99 ± 0.02	21 ± 1.5	0.29 ± 0.04
KBr	4.5	1.06 ± 0.03	28.8 ± 0.3	0.48 ± 0.05
KI	2	1.46 ± 0.04	6.5 ± 0.3	0.29 ± 0.07



Slow positron beam:

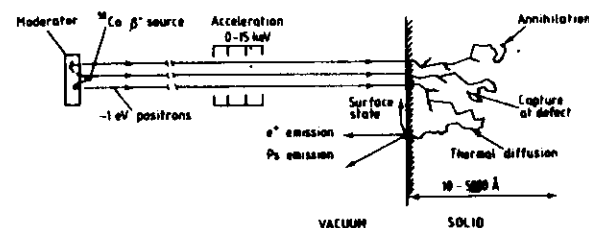


Fig. 9. Schematic view of a slow positron beam and positron surface processes.

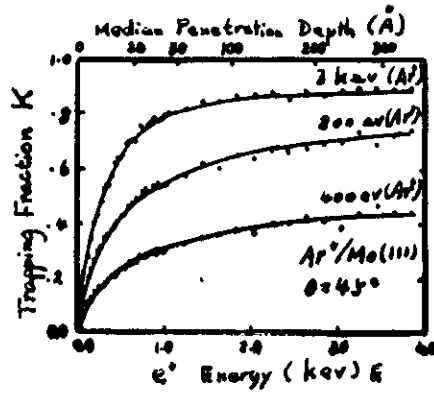
The thermalized positrons diffuse in the lattice

1. Annihilate as free particles.
2. Be trapped at a defect.
3. Reach back to the entrance surface.

The $3\tau/2\tau$ ratio gives an experimental measure to the fraction of Ps emission, which is proportional to the number of positrons diffused back to the surface.

Comparing the number of e^+ reaching back to the surface in the sample with and without defects one can deduce the fraction of trapped e^+ at various beam energies.

Ar⁺ sputtered Mo(111)



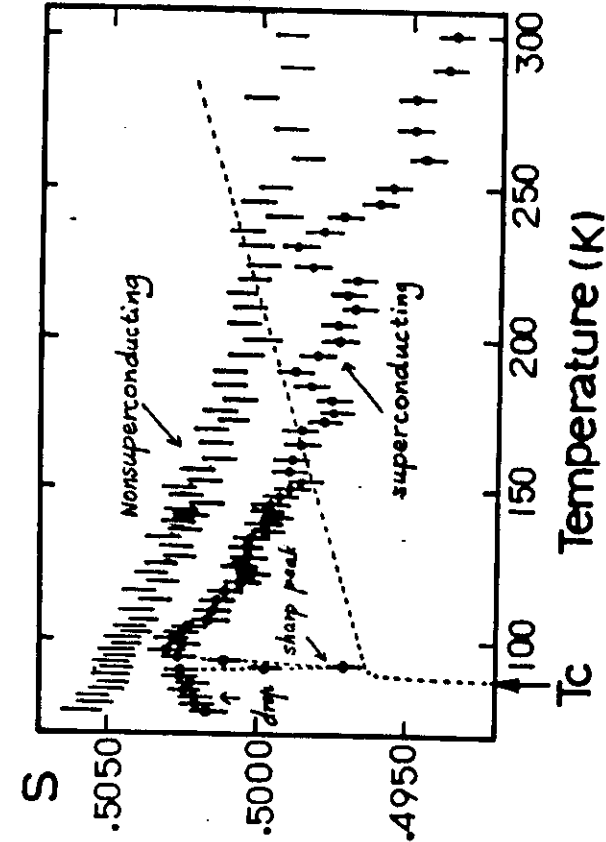
E: Positron beam energy

K(E): Fraction of trapped positrons

1. The mean positron implantation depth in Mo increases with incident energy.
2. At moderate energies, ($E > 1 \text{ keV}$), K also increases rapidly. (deeper depth)
3. At higher energies, K(E) becomes a constant. (defect distribution of finite depth)
4. The asymptotic value of K $\sim$ total number of defects integrated over the depth direction.

Zhang, Mao, Zhu, Lung, Proc. ICPA-8
(1988), Gent.

e⁺ in YBa₂Cu₃O₇₋₂



1. different temperature dependence near and below T_c (e⁺ delocalized between Cu-)
2. A sharp peak near T_c (also a internal friction peak). during structural transit
3. The complexity of the structure and questions of ionicity and covalency in the bonds in complex samples. (pure and simple structure samples needed.)

Fig. 2

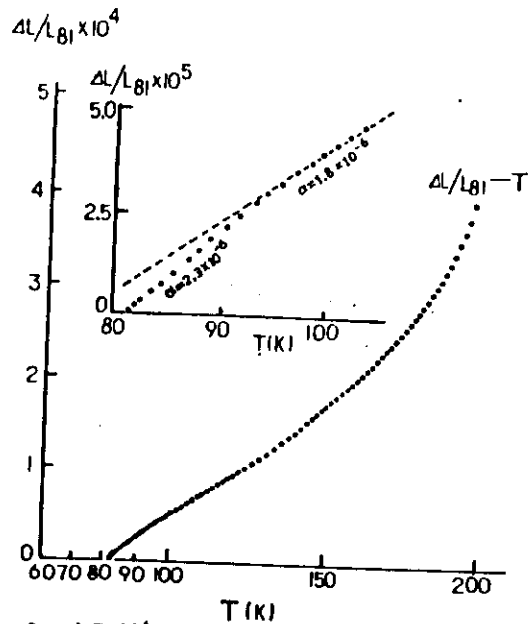


Figure 3. The $\Delta L/L_{B1}$ as a function of temperature in the range 80-200 K.

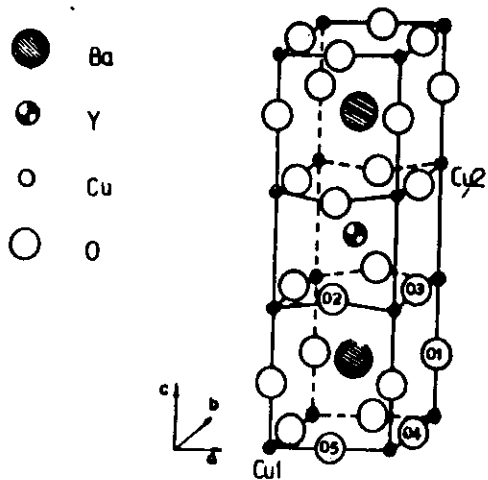


Figure 2. The crystal structure of $YBa_2Cu_3O_{7-x}$.

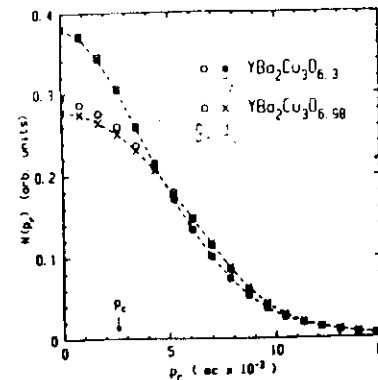


FIG. 1. Room-temperature radial distributions $N(p_r)$ of the 2D ACAR data for four $YBa_2Cu_3O_{7-x}$ samples described in text: crosses, A_1 ; circles, B_1 ; filled squares, C_{11} ; and open squares, D_{11} . $p_c = 2.6 \times 10^{-3}$ marks the cutoff momentum described in text.

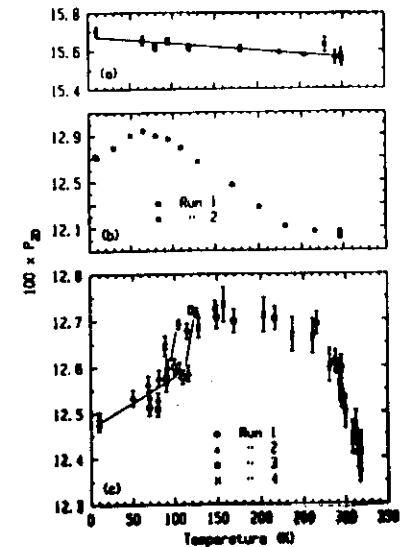


FIG. 2. Temperature dependence of the 3D shape parameter P_{3D} defined in text. (a) Nonsuperconducting sample D_{11} and the linear fit described in text. (b) Superconducting sample A_1 , for two warming cycles. (c) Superconducting sample B_1 , for four warming cycles; lines are drawn to guide the eye.

von Stetten, Berko, Li, Lee, et al.

High Sensitivity of Positrons to Oxygen Vacancies
and to Cu-O Chain Disorder in $YBa_2Cu_3O_{7-x}$
PRL, (1988), 2198.

ZHANG, ZHU, LUNG et al., Proc. ICPA-8, (1988) Gent.

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