Slow Positron Diffraction and Positron Holography

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Abstract

In this paper, we compare and contrast the scattering properties of slow positrons (20 eV to 300 eV) with that of low energy electrons. Particular emphasis is placed on the suitability of slow positrons in studying surface structure.

I. Introduction

It would be interesting to ponder why is the positron an ideal particle for studying surface structure? It is understood that an ideal probe for studying surface structure should have two basic attributes:

1) That the particle should have a very short mean free path (<10Å) so it is very sensitive to the top 3-5 atomic layers of a solid;

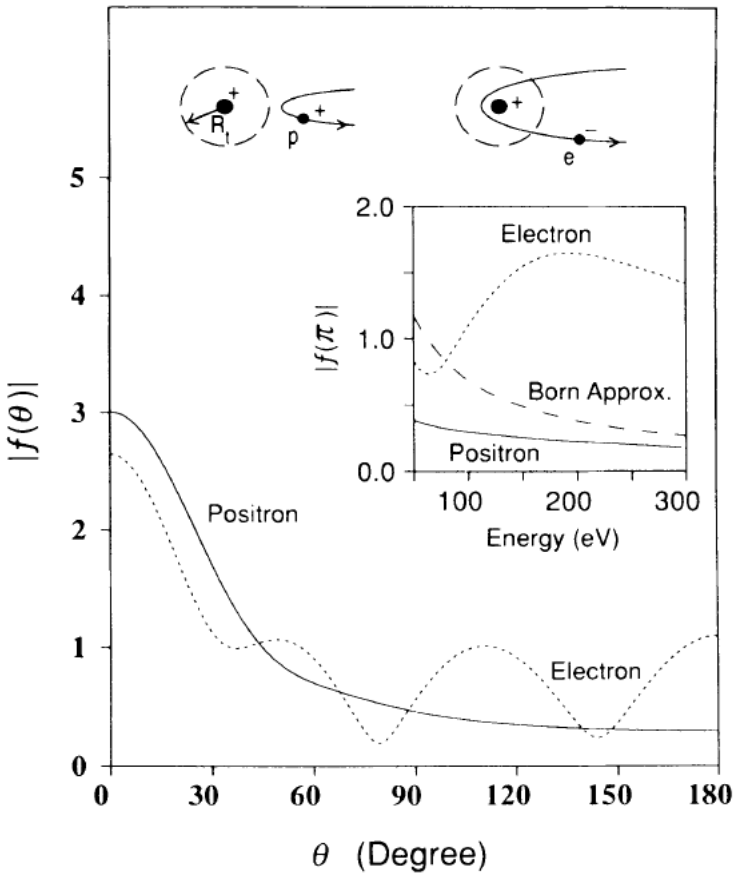
2) That the particle should scatter weakly with atoms so that the measured spectra can be easily simulated by theory or directly inverted to obtain structure.

If we consider the properties of slow positrons, we find that:

1) The mean free path of slow positrons (below 300 eV) in solids is shorter than that of electrons because there are no excluded final states for positrons in a solid. Therefore, slow positrons are even more surface-confined than electrons and thus, they provide detailed information of the surface within its top three to five atomic layers.

2) Because positrons are repelled by the atomic nuclei, the scattering of slow positrons by atoms resembles the Born approximation. See, for example, *Tong et al., PRL 69, 3654 (1992)*.

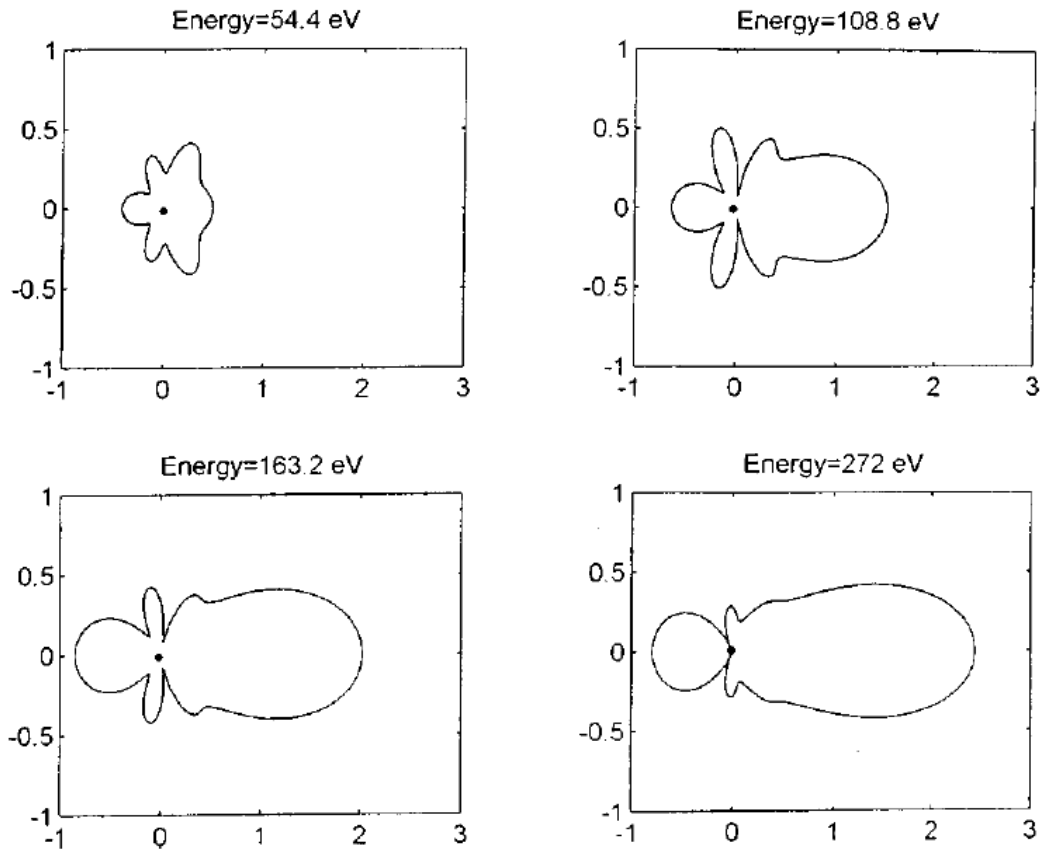
Figure 1 shows the scattering factor of electrons and positrons at 100 eV for Cu.



(Figure 1)

II. Properties of Electron Scattering

The scattering factor of slow electrons by atoms contains strong angular anisotropies [*Tong et al. PRB 58,10815 (1998)]*. Fig. 2 shows the electron scattering factor of Ni at various energies.



(Figure 2)

III. Lester Germer: The Father of LEED

Born : Chicago, 1896
1917 graduated from Cornell
1927 discovered low energy electron diffraction with S. G. Davisson

I met Lester Germer in the fall of 1969 when I arrived at Cornell University as a fresh postdoctoral associate. Germer at that time was a Fellow at Cornell University. He has retired from Bell Labs and was 73 then.

Germer and I spent many Saturday afternoons in my office drinking the bitter Carlsburg beer that he bought from India. Germer was looking for someone to develop a multiple scattering theory of LEED and I was looking for a new problem to work on. In March 1971, I published the first analysis of LEED using a new multiple scattering theory that I developed [*Tong and Rhodin, PRL 26, 711 (1971)]*.

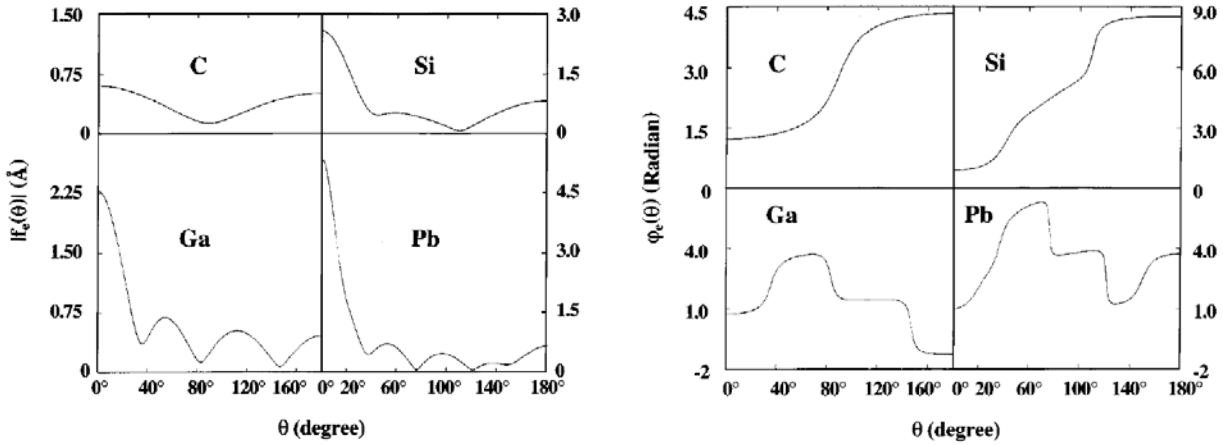
Germer was a vivid sportsman. He frequently walked from Ithaca to Syracuse (74 km). Unfortunately, Germer died in October that same year while he was rock climbing. I dedicated my essay " *Electron-diffraction for surface studies- the first 30 years*", *ed. C B Duke*, *North-Holland* 1994 to the memory of Germer, a true pioneer and my mentor in LEED.

IV. Origin of Electron Anisotropies

In 1998, I established two rules: For a given element, the maximum number of dips in the scattering factor $|f(\theta)|$ for electrons, positrons or x-rays equals (l+1) , where l is the highest bound orbital number.

At each dip of $|f(\theta)|$, its phase jumps by near π. [*Tong et al. Phys Rev B 58, 10815, (1998)]*.

Fig 3 shows electron angular anisotropies for C, Si, Ga at 100 eV and Pb at 300 eV.

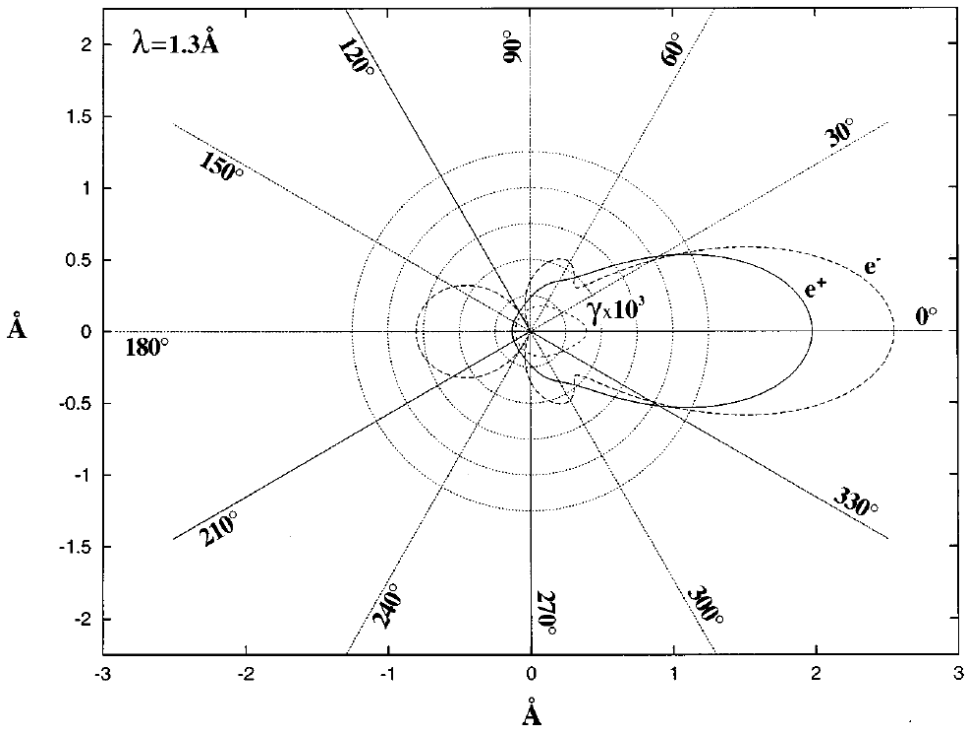


(Figure 3)

Atomic no. & Element	K 1 s	L 2 s p	M 3 s p d	N 4 s p d f	O 5 s p d f g	P 6 s p d ...
6 C	2	2 2				
13 Al	2	2 6	2 1			
14 Si	2	2 6	2 2			
26 Fe	2	2 6	2 6 6*	2		
28 Ni	2	2 6	2 6 8*	2		
29 Cu	2	2 6	2 6 10*	1		
31 Ga	2	2 6	2 6 10	2 1		
33 As	2	2 6	2 6 10	2 3		
47 Ag	2	2 6	2 6 10	2 6 10*	1	
74 W	2	2 6	2 6 10	2 6 10 14	2 6 4*	2
79 Au	2	2 6	2 6 10	2 6 10 14	2 6 10*	1
82 Pb	2	2 6	2 6 10	2 6 10 14	2 6 10	2 2

As there is no bound orbital for positrons and photons in atoms, there can be no angular anisotropy in their scattering factor. Fig 4 shows the radial plot of the magnitude of the scattering factor for electrons, positrons and photons at

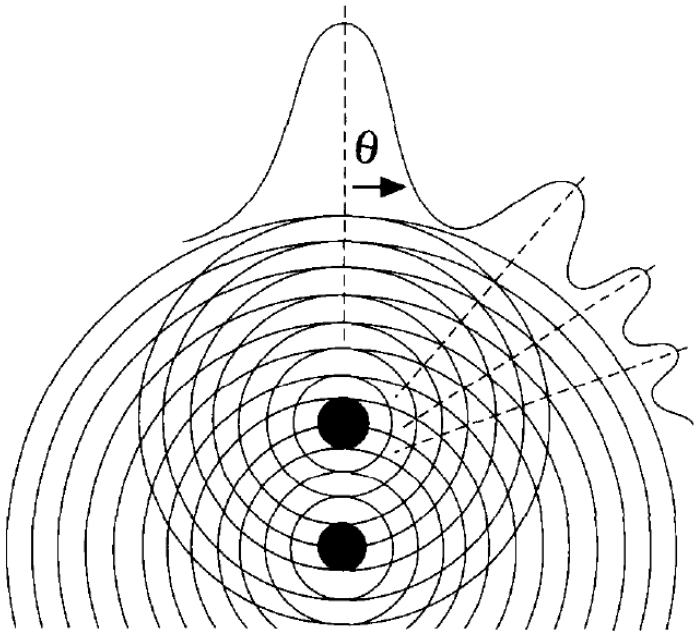
1.3 Angstrom wavelength. For the radial scale, each circular ring is 0.25 angstrom. [*Tong et al. Phys Rev B 58, 10815, (1998)*].



(Figure 4)

V. Forward Focusing (Slow Electrons) vs Forward Shadowing (Slow Positrons)

In the forward (zero angle) direction, the intensity enhancement factor is given by [*Poon and Tong PRB 30, 6211, (1984)*]:

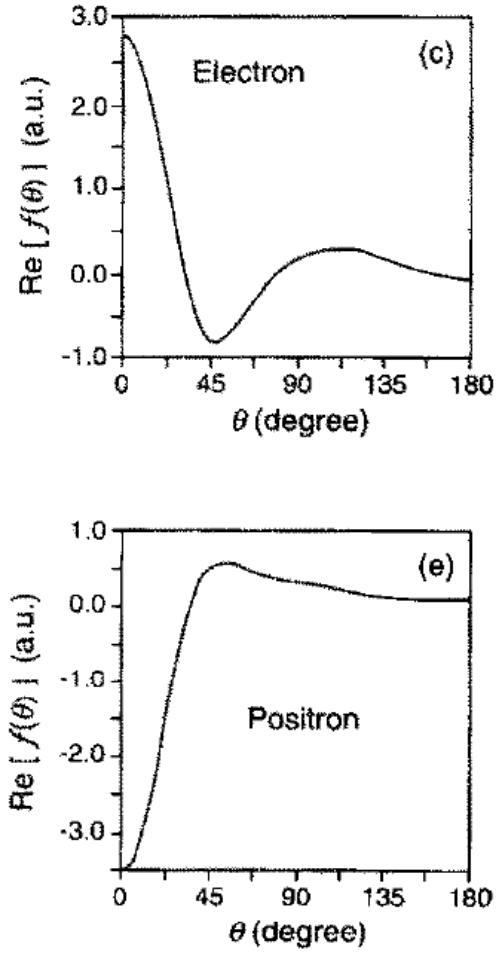


$$\chi(0) = \left(\frac{d\sigma}{d\Omega}\right)_{system} \Big/ \left(\frac{d\sigma}{d\Omega}\right)_{atom} = \left|1 + \frac{f(0)}{R}\right|^2$$

(Figure 5)

Because Re $f(0)$ is positive for electrons, $\chi_{electron}(0) = 3.14$

On the other hand, Re $f(0)$ is negative for positron scattering, $\chi_{positron}(0) = 0.36$ [*Li and Tong, Surf. Sci. Lett., 281, L347 (1993)*].



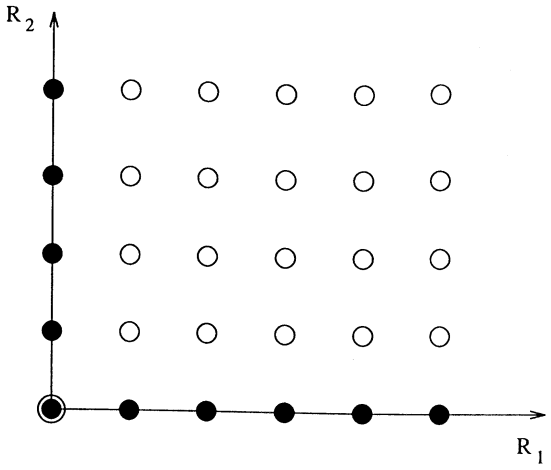
(Figure 6)

VI. Linear LEED vs Linear LEPD

The linear method [*Wander et al. PRB 46, 9897 (1992)*] searches for a global minimum in a "large" area (0.5Å x 0.5Å). It requires fully dynamical calculations at nN structures rather than N^n structures, where n is the number of *independent parameters* and N is the *number of variations* considered in each parameter.

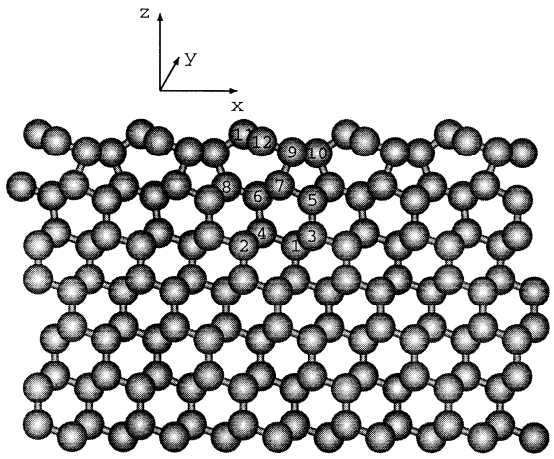
The amplitude in the linear approximation is given by:

$$A_L(\mathbf{r}_1', \mathbf{r}_2') = A(\mathbf{r}_1, \mathbf{r}_2) + A(\mathbf{r}_1', \mathbf{r}_2) - A(\mathbf{r}_1, \mathbf{r}_2) + A(\mathbf{r}_1, \mathbf{r}_2') - A(\mathbf{r}_1, \mathbf{r}_2)$$



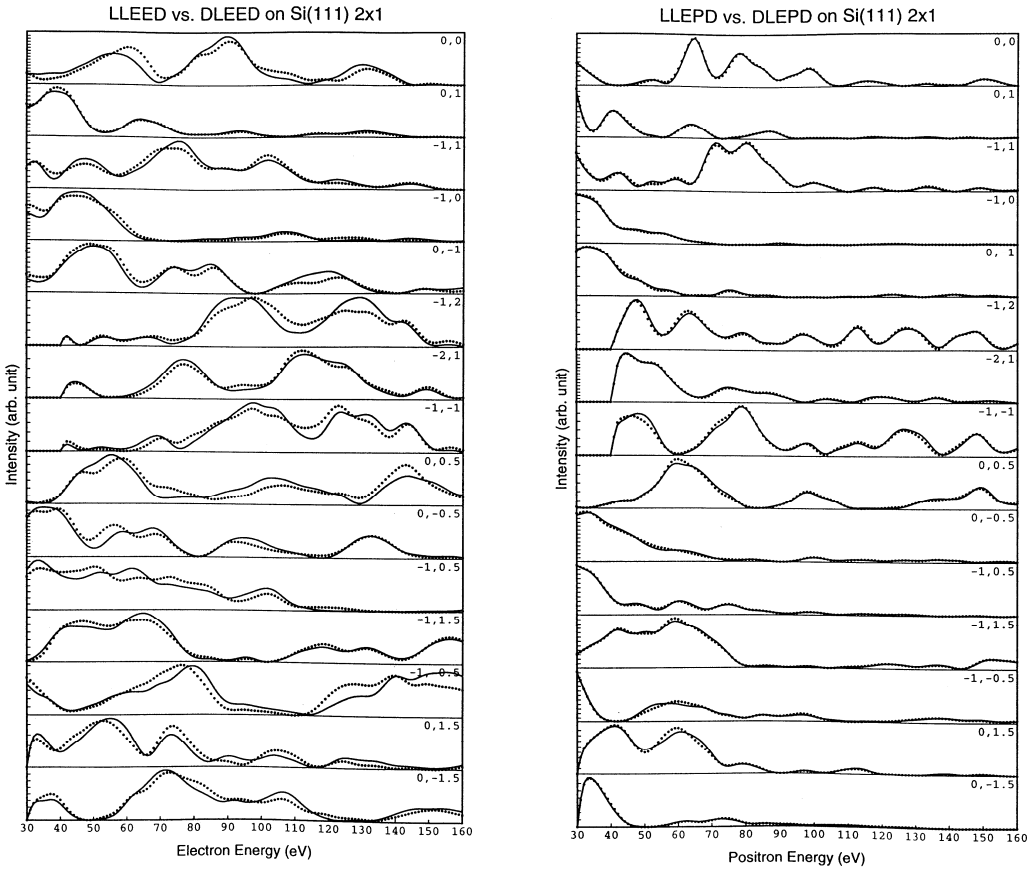
(Figure 7)

A test case for the linear method is the structure of the Si(111)-(2x1) pi-chain model. There are:
Number of variables: 36
36x5 calculations vs 5^{36} calculations (see fig 8).



(Figure 8)

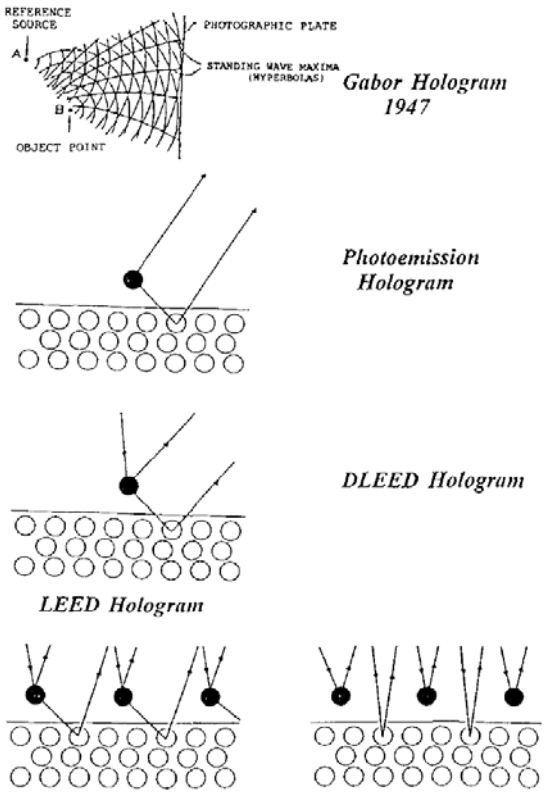
How well does the linear method work for LEED vs LEPD? [*S Y Tong SRL 7, 21 (2000)*]. Fig 9 shows results of linear method vs fully dynamical method for electrons (left) and positrons (right).



(Figure 9)

VII. Positron Holography: Inverting Experimental Data for Structure

Various forms of diffraction holography require that the scattering factor is "isotropic" and no sharp jumps in its phase. [*Tong et al. SRL 1, 303 (1994)*].



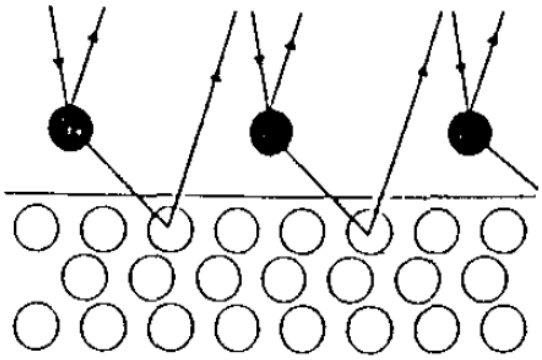
(Figure 10)

Inversion of diffraction data [*S. Y. Tong, Advances in Physics 1, 135, (1999)*] is given by*:*

$$\phi(\mathbf{R}) = \left| \int I(\mathbf{k_f}, \mathbf{k_i}) e^{i\mathbf{k_f}\cdot\mathbf{R}} d\Omega_{\hat{\mathbf{k}}_f} \right|^2$$

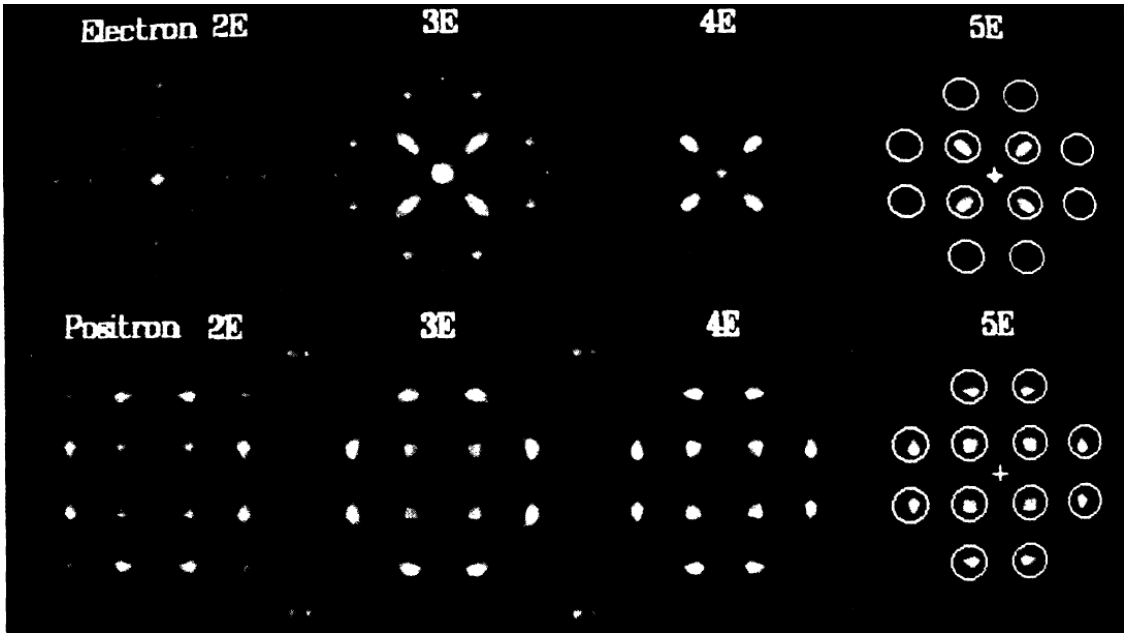
$$I(\mathbf{k_f}, \mathbf{k_i}) = |f_o^-(\mathbf{k_f}, \mathbf{k_i})|^2 + \cdots + f_o^{-*}(\mathbf{k_f}, \mathbf{k_i}) f_j^-(\mathbf{k_f}, \hat{\mathbf{R}}_j) \frac{f_o^+(\hat{\mathbf{R}}_j, \mathbf{k_i})}{R_j} e^{i(kR_j - \mathbf{k_f}\cdot\mathbf{R}_j)} + \cdots + \text{c.c.}.$$

LEED Hologram



(Figure 11)

The real space image for Cu(001) is shown in fig 12 [*Tong et al. PRL 69, 3654 (1992)*].



(Figure 12)

VIII. Conclusions:

Slow positron diffraction offers a number of unique properties, making this technique supremely suitable for studying surfaces.

Eighty five years after the discovery of low energy electron diffraction and twenty years after theoretical speculations about the merits of slow positron diffraction, the research at KEK and other similar facilities around the globe offer a long awaited “light” at the end of the tunnel.