Characterization of defects in ZnO implanted with Ar+ using positron annihilation technique

M Khulu [1], T Jili [1], M. Madhuku [2] and C Ndlangamandla[1]
[1]Physics Dept., University of Zululand, P/B X1001, Kwa-Dlangezwa, 3886
[2]iThemba LABS, Johannesburg, Gauteng

ABSTRACT

ZnO (wurtzite) samples were implanted with Ar+ ions to generate intrinsic defects within the samples for fluences ranging from 10^4 to 10^18 ions/cm^2. Doppler broadening of the annihilation centroids were obtained to determine S- and W - parameters which are associated with a quantity of defects. X-ray diffraction (XRD) method was employed to determine any structural or phase change associated with Ar+ implantation. The positron annihilation spectroscopy results were correlated with Optical absorption spectra of the crystals to investigate various bands at different fluencies. Theoretical calculations for potentials and wave-functions for both positrons and electrons were calculated. The electron-positron annihilation momentum density was also calculated for positron annihilations with core electrons up to low momentum electrons in valence states and vacancies.

[DUE TO LOCKDOWN AND DELAY FOR THE ARRIVAL OF SAMPLES, ONLY THEORETICAL APPROACH IS REPORTED IN THIS PAPER]

Method of calculation

- Annihilation rate, λ, is given by

$$\lambda = \pi r_o^2 c \int n_+(\boldsymbol{r}) n_-(\boldsymbol{r}) \gamma(n_-(\boldsymbol{r})) dr \quad (3)$$

γ(*n_(r))* is the enhancement factor in the Local Density Approximation (LDA) and in the Generalized Gradient Approximation (GGA). [1]

- the electron-positron momentum density in the so called state-dependent scheme [2] and given by

$$\rho(\mathbf{p}) = \pi r_o^2 c \sum_j \gamma_j \left| \int e^{-ip\cdot r} \psi_j(r) \psi_+(r) dr \right|^2 \quad (4)$$

$\psi_j(r)$ – jth state wavefunction

$\psi_+(r)$ – positron wavefunction

obtained from Linear Muffin Tin Orbital (LMTO) [2]

* Model the positron beam to determine depth profiles of positrons at different beam energies using Makhov profile equation:

$$P(z,E) = \frac{m z^{m-1}}{z_o^m} \, exp\left[-\left(\frac{z}{z_o}\right)\hat{}(m)\right]$$

With

$$z_o = \frac{AE^r}{\rho\Gamma(1+\frac{1}{m})}$$

Where

* A = 4.0 micro-gram cm^{-2} keV^{-r}

* m = 2, r = 1.6

* E is the positron beam energy

* Rho is the density of ZnO

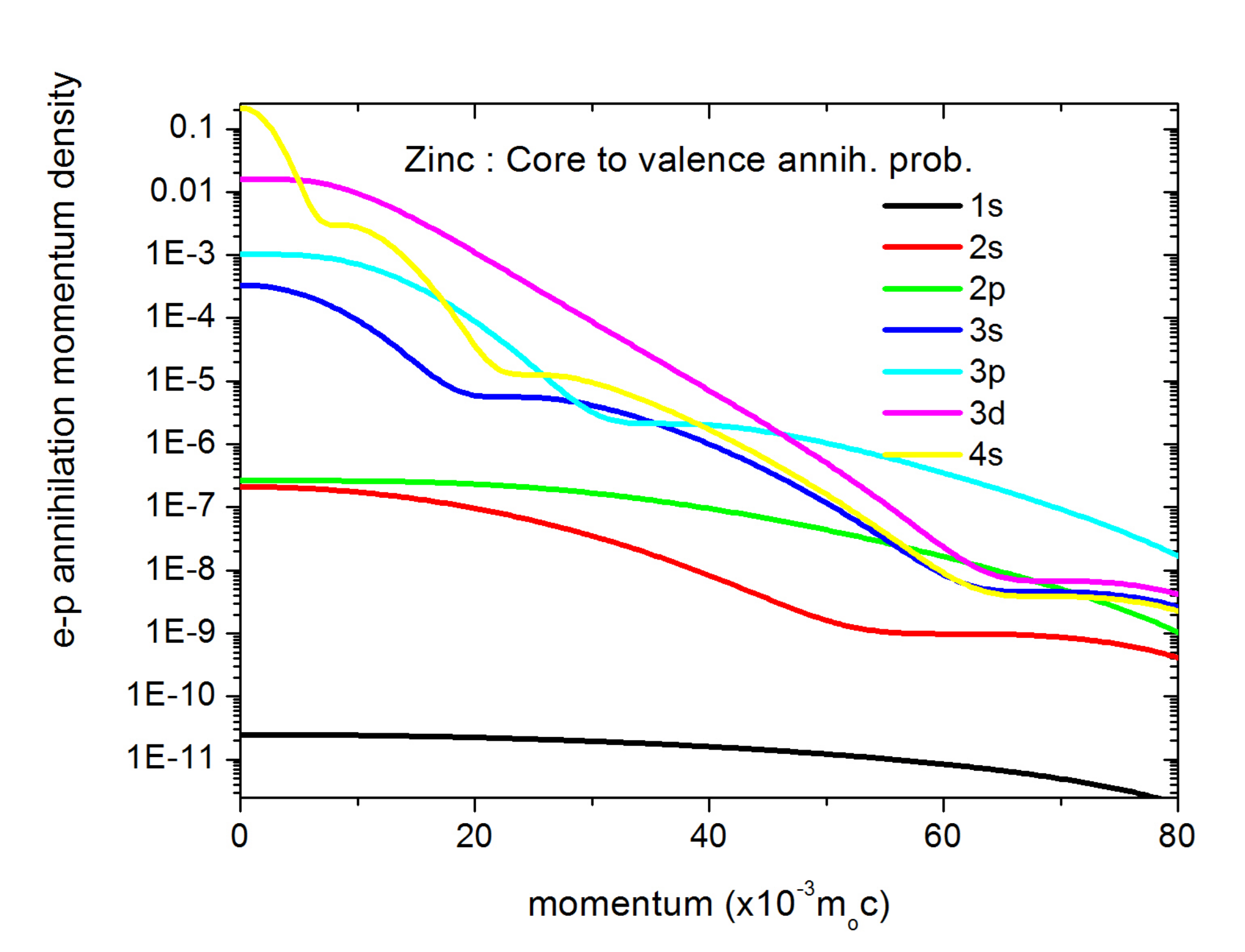

Figure 1. Positron-electron annihilations with core to valence states in Zinc. From (0-5)x 10^{-3} m$_o$c, 4s electrons dominate the annihilations with positrons at Zn vacancies. 3d electrons dominate between (5—47) x 10^{-3} m$_o$c.

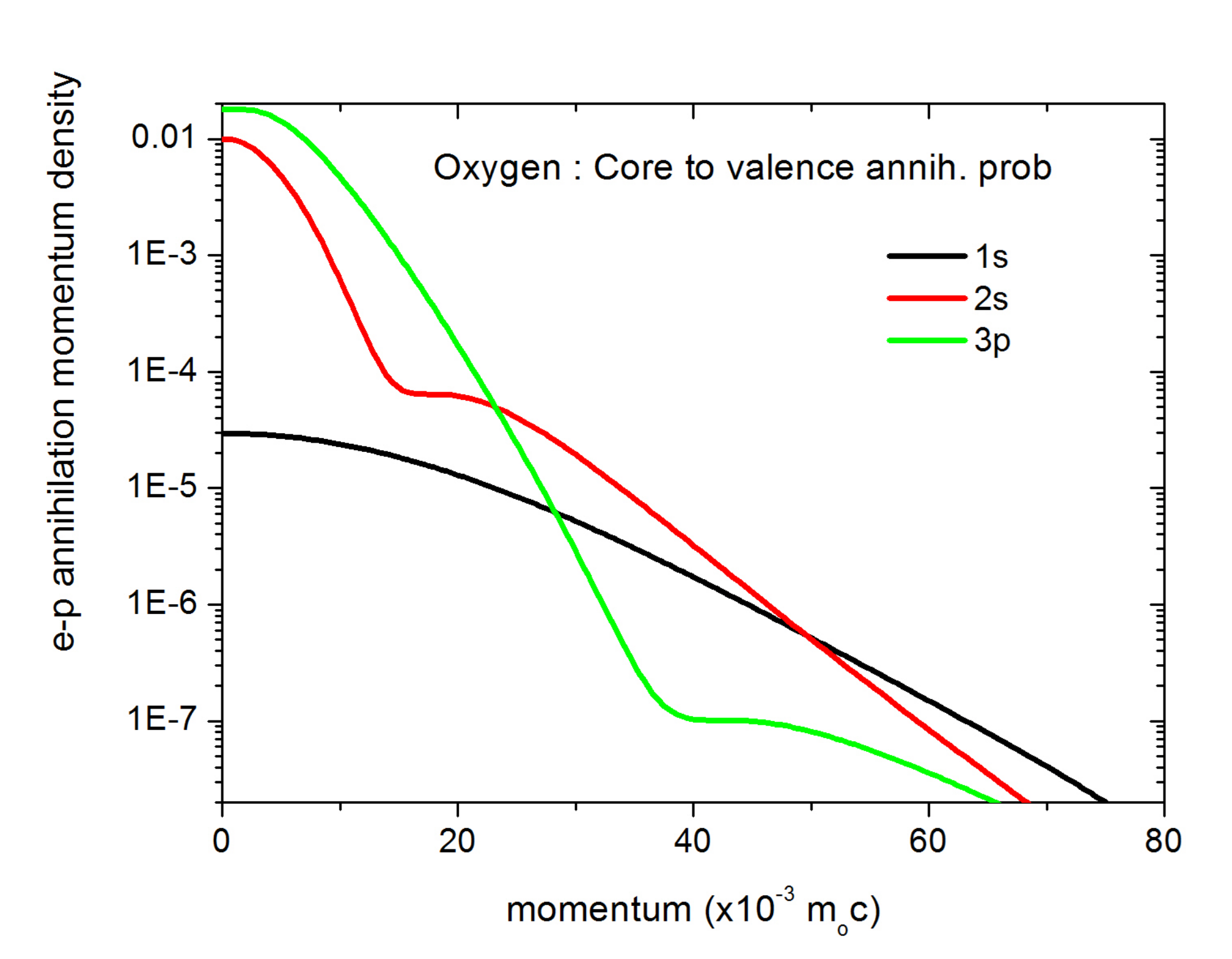

Figure 2. 3p electrons dominate the annihilations with positrons between (0—25) x 10^{-3} moc. These low momentum electrons contributes towards annihilations in the vacancies.

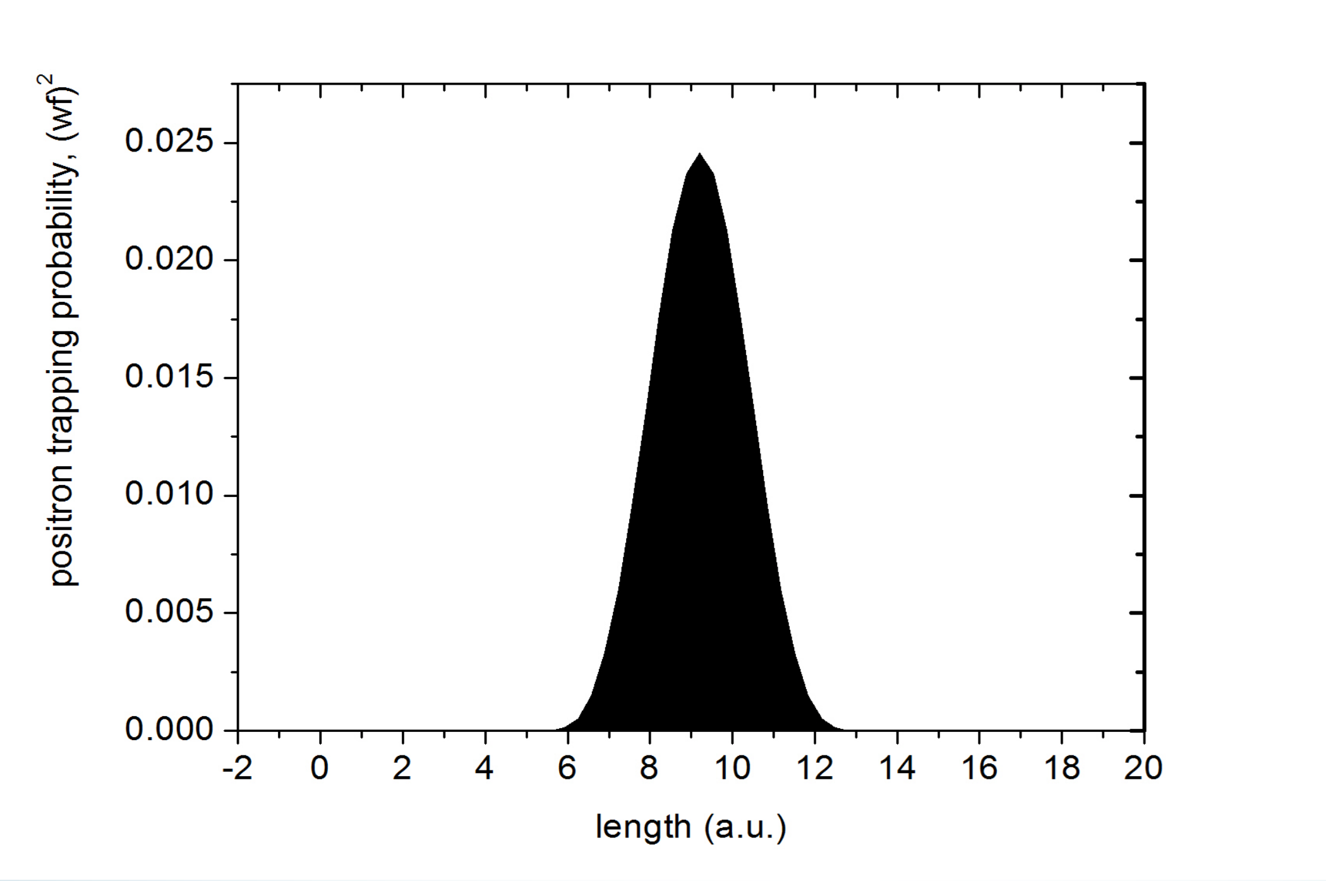

Figure 3 . The square of the wavefunction at Zn vacancy

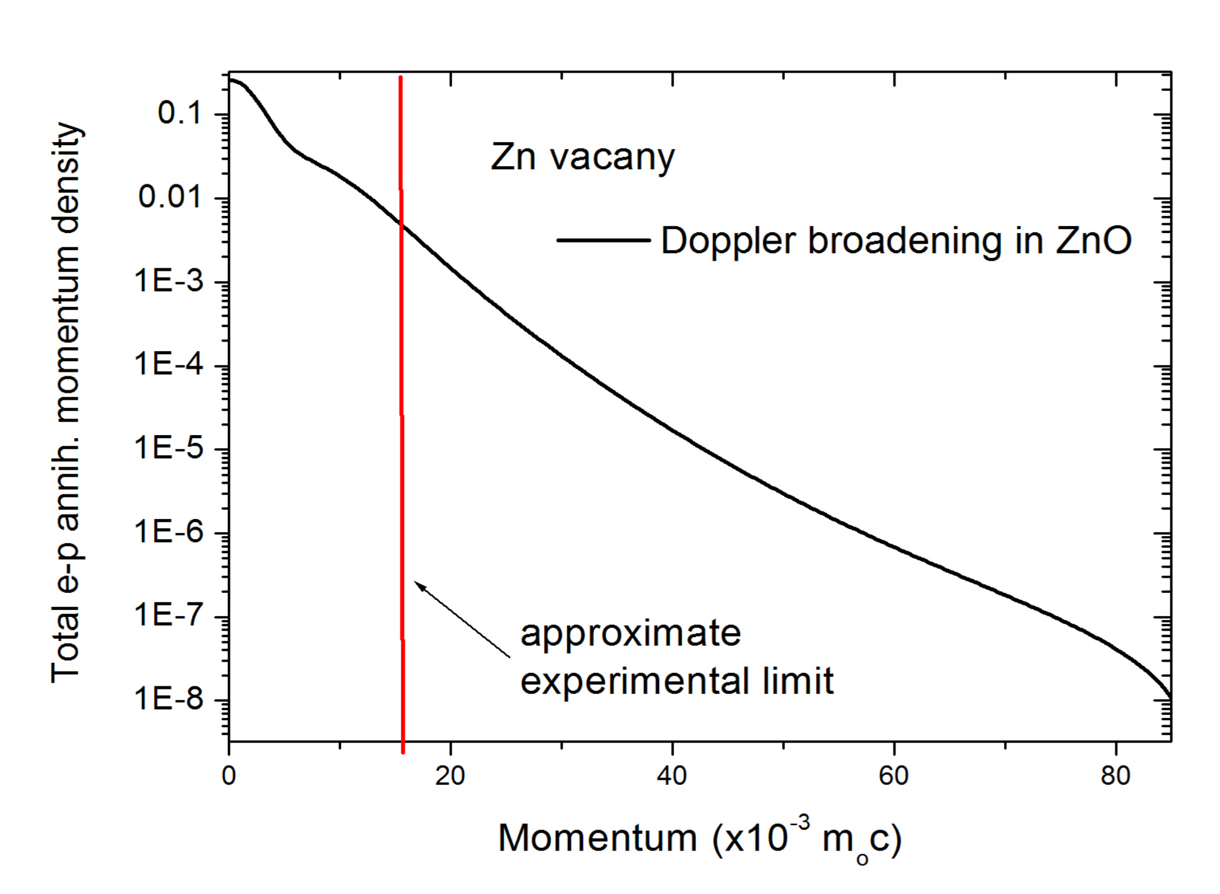

Figure 4. Total electron-positron annihilation momentum density [Doppler broadening] at Zn vacancy. The experimental procedure is also limited given the background noise

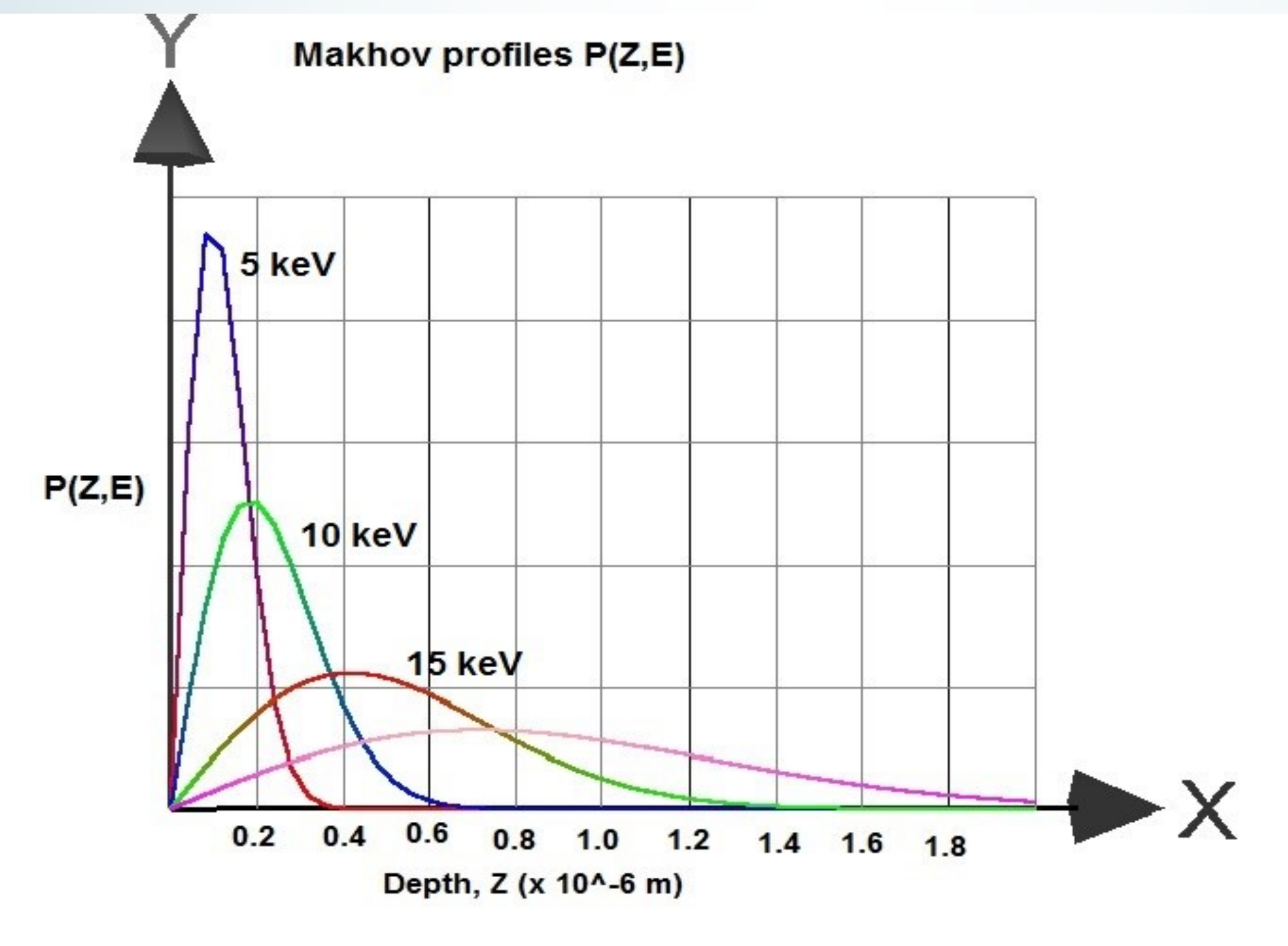

Figure 5. Makhov profiles in ZnO for positron beam at different beam energies 5, 10 , 15 and 25 keV assist in identifying the extent of radiation damage caused by ion-implantation

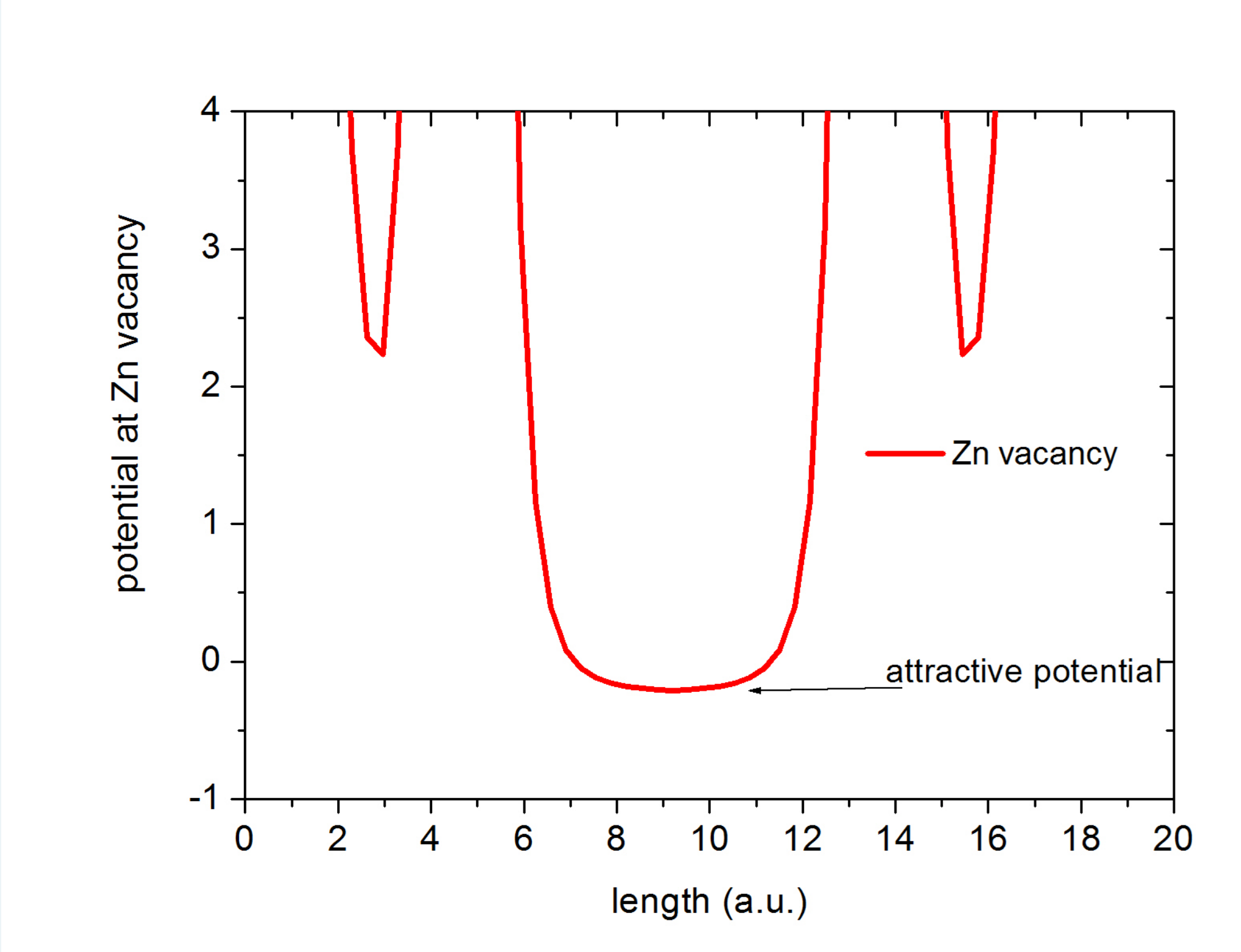

Figure 6. It is clear that the potential at Zn vacancy is favourable for positron trapping and annihilation

CONCLUSION

Although the experiment is not yet completed, the theoretical analysis based on LDA and GGA shows that Zn vacancies have sufficient potential to localize positrons for annihilations with electrons, figure 3 shows exactly the probability for a positron to be trapped in a Zn vacancy and the potential in figure 6 confirms the attractive nature (negative) of the Zn vacancy which makes it easy to trap the positron. The density of defects per ion implantation fluence is determined by knowing the depth profiles as shown in figure 5. Doppler broadening as shown in figure 6 is used to determine the concentration of defects. S-

REFERENCES

[1].Boronski E and Nieminen RN 1986 *Phys. Rev.* B34 3820

[2]. Nieminen RN and Manninen MJ 1979, *Positrons in Solids*, Springer-Verlag, Berlin, pg 143