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A Field-Assisted Moderator for Low-Energy Positron Beams

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Abstract. A new positron field-assisted (FA) moderator based on the drift of positrons across a cooled silicon crystal is proposed. Using estimates for both the β^+ implantation profile and attainable drift velocities, the efficiency of drift to a slow e^+ emitting surface is calculated using a diffusion equation which incorporates terms describing positron drift and annihilation. It is conjectured that efficiencies of up to 10% can be achieved. The use of epitaxially grown metallic silicide contacts to facilitate the application of the electric field is described and the consequences of using such contacts are fully discussed. Applications of the FA transmission mode moderator described here to produce timed brightness enhanced beams are briefly discussed.

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In a conventional moderator implanted positrons from a radioactive source rapidly thermalise and a small fraction can diffuse to a surface where, under favourable conditions, they can be emitted into vacuum with energies of a few eV. Following the initial conception of the positron moderator by Madanski and Rasetti [1] and the first practical demonstration by Cherry [2], the last 25 years have seen considerable improvement in conversion efficiencies. An important breakthrough was that of the MgO-smoked moderator with an efficiency of 3×10^{-5}, which enabled production of the first useful low-energy positron beam [3]. Further advances followed by the discovery of Mills that many clean metals in UHV emitted slow positrons [4] resulting in the development of higher-efficiency moderators [5]. The empirical relation for moderator efficiency can be written as [1, 6]

$$p = y_0 \mu \sqrt{D\tau} \tag{1}$$

with y_0 being the probability of positron emission from the surface, μ the absorption coefficient, and $\sqrt{D\tau}$ the e^+ diffusion length. In order to maximise these factors, work has recently concentrated on dense single-crystal metals with clean surfaces, especially W(110) for which an efficiency of 3.2×10^{-3} has been reported [7]. The importance of annealing in removing defects, which can lead to the trapping of e^+, has been realised.

Composite moderators have also been studied. For example, S on Cu(111) [8] has been found to improve efficiency as well as lessen the effect of exposure to air, and a thin layer of Cu(111) on W(110) [7] has enabled the combination of the high emission probability of Cu(111) with the superior stopping power of W.

Some improvements in the current technology have been suggested, for example the construction of a defect-free positron rectifier [9] and low-temperature cooling [10], but efficiencies greater than about 10^{-3} are unlikely since such moderators are mainly limited by the small fraction of the implanted positrons which diffuse to the moderator surface.

However, for an insulator or semiconductor the number of positrons reaching a surface may be enhanced by the application of an electric field. The concept

of field assisited (FA) moderation was first suggested by Lynn and McKee [11] who drifted positrons in a conventional Si surface barrier detector with a 200 Å gold window at the emitting face. They succeeded in only observing a very marginal increase in efficiency with increasing field and the overall efficiency was very low. Their apparent lack of success can be attributed to the existence of positron traps in the form of defects in the non-epitaxially grown gold contact and the presence of an SiO_2 "dead layer" between the Si(111) and Au.

We believe that these problems can be overcome by making use of epitaxially grown metal-silicide layers on a thin (50 μm) Si wafer. By cooling to 77 K efficiencies of up to 10% are predicted. This moderator would have the advantage of operating in transmission mode and it should be possible to collect fast timing pulses from the positrons as they thermalise in the semiconductor bulk.

In this paper we give the theoretical basis for such a moderator. Section 1 deals with implantation of fast positrons, Sect. 2 with the solution of the diffusion equation with electric field drift and in Sect. 3 the effect of a thin silicide barrier on the emitting face is considered. Finally, in Sect. 4 the possibility of using a Si moderator for brightness enhancement is discussed.

1. Implantation

An accurate knowledge of implantation profiles has been of increased importance recently with the aim of optimising transmission moderator thicknesses to achieve greater conversion efficiencies. An important point is that in theoretical calculations the implantation profile is usually taken to be the time equal 0 boundary condition for the solution of the relevant transport equation used to describe the subsequent motion of the thermalised positron [12].

It has been established experimentally that β^+ stopping profiles are close to exponential in form, although an adequate theoretical explanation has yet to be offered. The profile can therefore be written as

$$p(x)=\mu\exp(-\mu x), \tag{2}$$

where μ, the absorption coefficient, can be written as

$$\mu=\varrho\alpha \tag{3}$$

with α being the mass absorption coefficient and ϱ the target density. α has been shown to obey the empirical formula [13]

$$\alpha=1.7T_E^{-1.14} \tag{4}$$

where T_E in MeV is the β^+ endpoint energy (0.545 MeV for [^{22}Na). For ^{22}Na this gives a value of $\mu=7909\ \mathrm{m}^{-1}$ for Si, in good agreement with the experimental measurement made by Brandt and Paulin [14] after correction for the different endpoint energy of their β^+ source used (^{64}Cu). The result, however, disagrees with that determined from the Z-dependent expression given by Mourino et al. [15]. The reason for this disagreement is not known.

In order to verify the value for μ, a Monte Carlo simulation was performed. Apart from a 10% increase in range for positrons over electrons, it was noted that $\beta^\pm$ profiles are very similar, so a range energy relation for positrons in Si was parameterized from the corrected electron data of Erginsoy et al. [16] and was found to be conveniently written as

$$\ln(r)=7.478+1.625\ln(T)-0.0954\ln^2(T), \tag{5}$$

where r is the mean radial distance in μm travelled by a positron of kinetic energy T in MeV. In the simulation, positron energies were weighted according to the ^{22}Na spectrum and the probability of the radius vector making an angle θ relative to the normal of the moderator (Fig. 1) given by the solid angle available for that angle assuming isotropic implantation from the source. 140 000 events were stored according to the planar implantation depth, x, given by $r\cos\theta$. The resulting profile is shown in Fig. 2. The most important feature of the resulting distribution is the exponential variation over the range 60–250 μm with an absorption coefficient ($\mu=7892\pm34\ \mathrm{m}^{-1}$) in good agreement with (3) and the result of Brandt and Paulin [14]. At distances >250 μm deviations from the exponential are observed. This is expected as it is known that the profile does not extend beyond a certain range but this

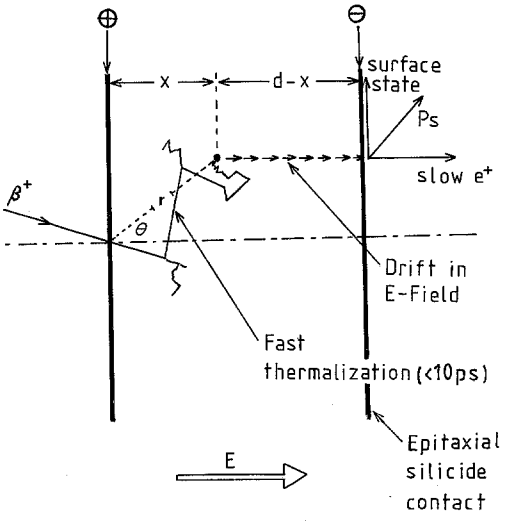

Fig. 1. A schematic diagram of the field-assisted silicon moderator. The positron thermalises within 10 ps to a position (r, θ), and implantation depth $x=r\cos\theta$. It then drifts in the applied E-field towards a thin (20 Å) epitaxial silicide contact where it is emitted into vacuum

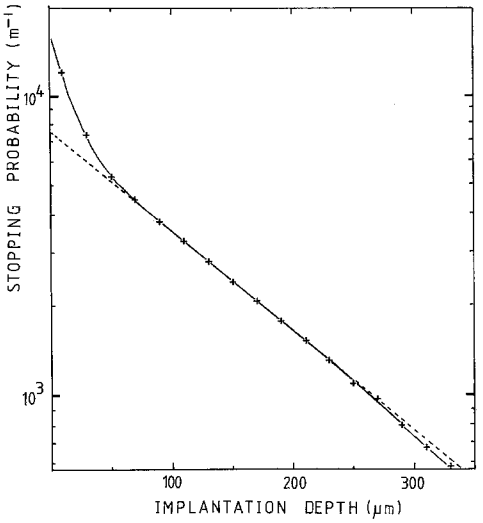

Fig. 2. The stopping profile of ^{22}Na positrons in silicon based on a Monte-Carlo simulation of the slowing down process. The dotted line represents the best exponential fit to the data between 70 and 250 μm

is of no concern here since it is greater than any practicable drift distance. At distances $<60\,\mu m$ the results are above the exponential profile. This is probably due to the θ variation allowed for in the simulation. Recently Vehanen and Makinen [17] made a similar study, in which they convoluted the Makhov profile for monoenergetic impact with the ^{22}Na spectrum and obtained profiles for Cu and Al, which, below about 10 μm, were less than the exponential profile. However, direct comparison of these results with those of the present study is not possible since they assumed collimated implantation with no θ variation. Experimentally, little difference between collimated and isotropic implantation is observed, presumably because the collimated beam rapidly becomes isotropic on entry into the material [13]. This loss of collimation would depend on the Z-value of the material and differences might be more apparent in lower Z materials like Si and Al. Unfortunately, collimated-slit experiments [15] at present lack the resolution to investigate profiles at depths less than about 100 μm.

Another important point is that, in practice we do not have the ^{22}Na spectrum of β^+ because of the effect of backscattering of the positrons from the source mount. 50–60% of backward emitted positrons can, by this process, be implanted into the moderator at a lower energy [18]. This effect is not considered here in detail: it is merely noted that its action will be to increase the expected yield over those predicted here.

Distortion of the implantation profile as a result of the applied field can be shown to be negligible. Jorch et al. [19] treat thermalisation in semiconductors as a 2 stage process consisting of a fast sub-picosecond slow down to the band gap energy by electronic excitations followed by a slower phonon emission process taking 6 ps if the positron is to cool to a lattice temperature of 77 K. With an electric field applied, positrons will not reach thermal equilibrium but the time scale of the process allows us to estimate that positrons will at the most drift an additional 0.5 μm during thermalisation and that only about 1% will annihilate.

With the uncertainties surrounding the exact nature of the profile, we decided to adopt two profiles in this study:

1) the exponential profile of (1) with $\mu^{-1}=127\pm3\,\mu m$ and

2) the profile obtained from the Monte-Carlo simulation.

2. Positron Transport in an Electric Field

For most practical cases, positron drift and diffusion in a moderator can be adequately described by solving the diffusion equation which, for a one-dimensional problem, takes the form

$$\frac{\partial n(x,t)}{\partial t}=D\frac{\partial^2 n(x,t)}{\partial x^2}-v\frac{\partial n(x,t)}{\partial x}-\lambda n(x,t)\,, \tag{6}$$

where $n(x,t)$ is the positron probability density and D, v, and λ are, respectively, the diffusion coefficient, drift velocity and decay rate of the positron.

Several authors (Mills and Murray [20], Sferlazzo [21], Vehanen et al. [17] and Jorch et al. [19]) have obtained solutions to (6) subject to various boundary conditions. Here, we give an exact solution to the equation for an exponential positron implantation profile into a moderator of thickness d and sustaining an electric field E subject to the following boundary conditions

$$\begin{aligned} &n(0,t)=n(d,t)=0\,,\\ &n(x,0)=\mu\exp(-\mu x)\qquad (0<x<d)\,. \end{aligned} \tag{7}$$

Combining (6 and 7) we obtain

$$\begin{aligned} n(x,t)=\frac{2\pi\mu}{d^2}\sum_{n=1}^{\infty}&\frac{n}{[\mu+(v/2D)]^2+(n\pi/d)^2}\\ &\times[1-(-1)^n\exp\{-[\mu+(v/2D)]d\}]\\ &\times\exp\{-[(n\pi/d)^2D+\lambda+D(v/2D)^2]t\}\\ &\times\sin(n\pi x/d)\cdot\exp(vx/2D)\,. \end{aligned} \tag{8}$$

From (8), the probabilities $q(0)$ and $q(d)$ of the positrons diffusing to the surfaces at $x=0$ and $x=d$, respectively, can be determined as

$$q(0)=\int_0^\infty D\frac{\partial n}{\partial x}\bigg|_{x=0}dt\,,\qquad q(d)=-\int_0^\infty D\frac{\partial n}{\partial x}\bigg|_{x=d}dt \tag{9}$$

and yield

$$q(d)=\frac{\mu\exp(vd/2D)}{d[(\lambda/D)-\mu^2-(\mu v/D)]}\left[\frac{a}{\sinh a}-\frac{b}{\sinh b}+e^{-a}(b\coth b-a\coth a)\right]$$

$$q(0)=\frac{\mu}{d[(\lambda/D)-\mu^2-(\mu v/D)]}\left[b\coth b-a\coth a+e^{-a}\left(\frac{a}{\sinh a}-\frac{b}{\sinh b}\right)\right]$$

with

$$a=\mu d+(vd/2D)$$

and

$$b=d[(\lambda/D)+(v/2D)^2]^{1/2}. \tag{10}$$

To operate a field-assisted moderator efficiently, we need to be in the regime where the drift distance is significantly greater than the diffusion length. The condition for this is

$$v\gg\sqrt{2D\lambda}.$$

Substituting some physical values ($\lambda=4.55\times10^9\,\mathrm{s}^{-1}$ (22); $D=3.2\times10^{-4}\,\mathrm{m}^2\,\mathrm{s}^{-1}$ [23]) gives

$$v\gg1\times10^3\,\mathrm{ms}^{-1}.$$

In this case the quantities $q(d)$ and $q(0)$ reduce to

$$q(d)=\frac{\exp(-\mu d)-\exp(-\lambda d/v)}{(\lambda/\mu v)-1},\qquad q(0)=0. \tag{11}$$

Before using these results to calculate moderator efficiencies, it is necessary to estimate positron drift velocities in Si. The only experimental results are those of Mills and Pfeiffer [23] who, at low electric field ($<6\,\mathrm{kV\,cm}^{-1}$), obtained mobility values, u_+, of 460 and $173\,\mathrm{cm}^2\,\mathrm{v}^{-1}\,\mathrm{s}^{-1}$ at 80 and 184 K, respectively, thereby clearly demonstrating the temperature dependence of this parameter. With some degree of certainty the data can be fitted to Shockley's [24] theoretical expression for acoustic phonon limited drift velocity

$$v=\sqrt{2}u_+E\{1+[1+(3\pi/8)(u_+E/v_1)^2]^{1/2}\}^{-1/2},$$

where E is the applied electric field and v_1 the longitudinal sound velocity, $v_1=8.43\times10^3\,\mathrm{ms}^{-1}$ in Si. This expression can be extrapolated to high fields, where it has been established that electron drift velocities saturate at about $10^5\,\mathrm{ms}^{-1}$, due to optical phonon interactions. Mills and Pfeiffer [25] suggest that positron velocities are also limited by optical phonon scattering and saturate at a similar value. Using (13), it is estimated that at 80 K saturation will occur at fields approaching $100\,\mathrm{kV\,cm}^{-1}$. It should be noted that, although the breakdown field strength for Si is about $300\,\mathrm{kV\,cm}^{-1}$, contact failure may occur at smaller fields. This point is discussed further in the next section.

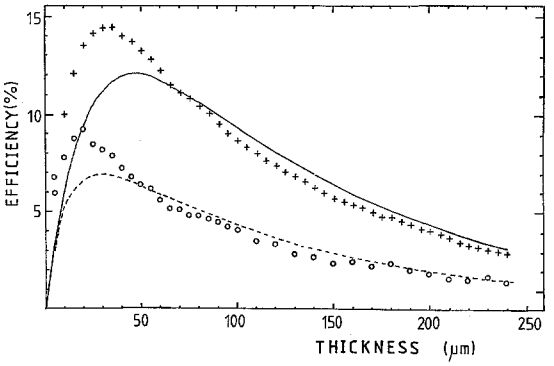

Fig. 3. Calculated efficiencies as a function of moderator thickness assuming perfect emission from the silicide contact. —— $v=10^5\,\mathrm{ms}^{-1}$, – – – $v=5\times10^4\,\mathrm{ms}^{-1}$ (exponential stopping profile, (11), + + + $v=10^5\,\mathrm{ms}^{-1}$, ooo $v=5\times10^4\,\mathrm{ms}^{-1}$ ms^{-1} (Monte Carlo, 140 000 events).

Figure 3 shows plots of transmission efficiency against moderator thickness for several different drift velocities using both an exponential profile and that obtained from the Monte-Carlo simulation. In the latter case the probability of positrons reaching the surface was weighted according to their survival probability, $\exp[-\lambda(d-x)/v]$. Results suggest that efficiencies in excess of 10% are feasible, although this may not be realised experimentally due to the electrical silicide contact layer. This point is discussed further below.

3. Transmission Through the Silicide Contact

Although emission of positrons from a Si(111) surface has been observed experimentally [26], work by Shultz et al. [27] shows that even a few monolayers of Cu(111) on a W(110) moderator changed the work function to that of Cu(111). The choice of material for the front contact of the FA moderator is therefore critical to the success of the device. This, together with the work of Lynn and McKee [11] suggests that the contact should be epitaxially grown and should have a negative work function less than that of Si(111) (1 eV).

It is suggested that these requirements can probably be met by forming a thin epitaxial silicide contact on the Si(111) surface. Four silicides are known to form epitaxially on Si(111) and these are $NiSi_2$ [28], $CoSi_2$ [29], PtSi [30], and Pd_2Si [31]. These compounds have been shown to form Schottky barriers of precise

and reproducible height on both n- and p-type Si [32]. In the former case depletion occurs from the emission surface where the largest fields are appropriate. For intrinsic material, the resulting nature of the interface will limit leakage currents to less than 10^{-10} A at 77 K [33], so there will be negligible voltage drop along the contact, which would otherwise result in an energy spread of the emitted positrons.

Positron transmission through the silicide is expected to be close to 100% efficient; the y_0 value of the Si(111) being replaced by that of the silicide. If quantum mechanical reflection at the step down in potential occurs, the electric field will drift the positron back towards the barrier, increasing the implantation probability to near 100%. Providing the contact is thin enough (< 50 Å) in comparison to the positron diffusion length in the silicide, the rectifying action of the potential step will ensure almost 100% diffusion to the surface once in the silicide. Moreover, because of themalisation and zero-field conditions within the contact the emission of e^+ from the silicide will be characteristic of the lattice temperature, rather than the positron temperature within the Si. The latter is limited by optical phonon scattering to a temperature of 800 K. In this sense the contact is advantageous as it is known that low temperatures improve the forward emission and energy spread of e^+ from flat crystalline surfaces [34].

The magnitudes of electric fields that can be sustained within what is effectively a fully depleted surface barrier detector are found to be limited by the rear contact which is usually ohmic and made of aluminium. Breakdown usually occurs at fields around 25 kV cm^{-1} due to minority carrier injection [35]. This problem could be overcome by replacing this contact with a second silicide layer on a well polished surface. Fields approaching 100 kV cm^{-1} resulting in the saturation of the positron velocity can then be applied. There is also some indication that strong inherent electric fields can arise at Si surfaces if the substrate is annealed to high temperatures (> 1300 K) to remove sputter damage [36]. However, work by Nielsen et al. [37] suggests that if lower temperatures (1100 K) are used this effect can be avoided.

Thin (20 Å) $NiSi_2$ layers can be grown with a uniformity of ± 7 Å by annealing a thin Ni layer for 5 min at 800 K [38]. UHV is necessary if good quality, pure films are to be made. Results show that these films are dislocation free, form atomically abrupt interfaces and have a negligible number of disordered Ni atoms at the interface. Should the epitaxial silicides not prove suitable polycrystalline silicides such as WSi_2 and $MoSi_2$ could be tried. These have grain sizes of about 1000 Å, which is about the magnitude of the positron diffusion length in metals.

Although Si(111) is the initial choice for a FA moderator, it is worth noting that Al can be grown epitaxially onto GaAs (100) [39] and that Al emits slow positrons with an energy of 0.19 eV [40], although the workfunction of GaAs is not yet known. This could provide the basis for a future FA moderator experiment.

4. Brightness Enhancement Using FA–Si Remoderators

The process of brightness enhancement [41] involves electrostatic focussing of a beam by acceleration to 5–10 keV, followed by remoderation leading to a secondary beam of substantially increased brightness/volt. If the remoderator thickness is optimised for the monoenergetic incident beam, losses at this stage are small. Brightness enhancement using reflection mode geometry has been accomplished [34], but use of transmission moderation has the distinct advantage of separating the electrostatic optics required for incident and remoderated beams.

A FA moderator of the type already described in this paper, but made to a thickness of < 5 μm is seen to be an ideal transmission remoderator. With an incident beam of 10 keV and a positron drift velocity of 10^5 ms^{-1} in the Si wafer nearly 100% transmission of positrons is possible. Figure 4 shows calculated transmission probabilities for a FA–Si(111) moderator assuming drift velocities of 0.1, 0.2, 0.5, and 1×10^5 ms^{-1}, based on the Makhov implantation profile parameters $A = 206$ Å/keV^{-n}, $n = 1.6$, and $m = 1.9$ as used by Nielsen et al. [37] for Si. In these calculations we have ignored the effect of the silicide

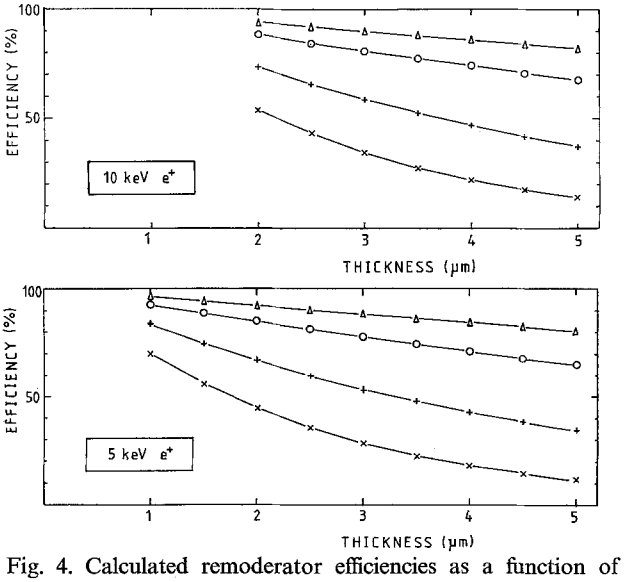

Fig. 4. Calculated remoderator efficiencies as a function of thickness assuming perfect emission from the silicide contact. Δ $v = 10^5$ ms^{-1}, ○ $v = 5 \times 10^4$ ms^{-1}, + $v = 2 \times 10^4$ ms^{-1}, × $v = 10^4$ ms^{-1}

layer, but we note that even if this reduces the efficiency by a factor of 5, a FA–Si(111) remoderator will be as good as the best 1000 Å W(100) foils, which have an efficiency of 18% [42].

The FA–Si(111) remoderator has the practical advantage over thin foils of being self-supporting in vacuum due to its greater thickness. There is also the added advantage that it is essentially a fully depleted surface barrier detector, similar to those normally used in ΔE measurements of heavy ionizing particles in nuclear spectroscopy, and can therefore furnish a small but fast charge collection pulse, which could be used to time the beam. Using this type of detector Petersen [43] has been able to detect electrons of energies < 5 keV using optimal charge sensitive amplification.

In contrast to a primary FA moderator, energy loss in the entrance window may now be of significance. It is therefore proposed that both contacts should be thin silicides. An additional benefit is that the remoderator could be grown as a heterostructure [44]. Starting with a Si(111) substrate a 20 Å $CoSi_2$ + 2 μm Si(111) + 20 Å $CoSi_2$ structure could be grown by MBE or thermal annealing. The substrate can then be removed by chemical etch or sputtering to yield the remoderator.

5. Conclusions

The field assisted (FA) moderation principle as applied to a Si(111) single crystal has been fully described. The main difficulties in constructing this type of moderator stem from the lack of present knowledge about the e^+ emission properties of the epitaxial silicide contacts. Experiments are presently underway at UCL, aimed at characterising the surface emission from epitaxial silicides, with the aim of producing a FA–Si(111) moderator. If an efficiency close to 10% can be achieved it will be possible to produce beams of 10^8–10^9 e^+s^{-1} in the laboratory without having to resort to high flux reactors [45] or LINACS [46], which are currently the only means of producing these intensities. Moreover, there would be significant advantage in being able to produce efficient timing transmission remoderators.

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