Optimization of superconducting tunnel junction based x-ray detectors

C. L. Foden, N. Rando, A. Peacock, and A. van Dordrecht
Astrophysics Division, Space Science Department of the European Space Agency, ESTEC, Noordwijk, The Netherlands

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Current research into x-ray detection using superconducting tunnel junctions indicates that the poor spectral resolution obtained so far, in comparison with theoretical expectations, is partly due to the excellent acoustic coupling of the junction and substrate. The substrate acts both as a source of noise and as a heat sink for the nonequilibrium junction, thus masking the intrinsic response of the superconducting electrodes to photoexcitation. A new design for a superconducting tunnel junction based on an x-ray detector is presented. The design effectively decouples the substrate and junction and should therefore eliminate many causes of spectral degradation, bringing resolution closer to that predicted theoretically, and thus allowing experimental investigation of the intrinsic superconducting film response to x-ray photoexcitation. An outline of the way in which the design can be optimized geometrically to achieve the decoupling is given. Further optimization of the intrinsic film response to x-ray photons is achieved through the introduction of specific absorbing and trapping regions to improve both the quantum efficiency and charge output of the new design. The use of "pairing potential barriers" within the electrode leads will also improve the intrinsic resolution of this device.

I. INTRODUCTION

In recent years, the search for improved resolution in x-ray detection systems has led to increased use of superconducting materials as the key element in both readout and absorbing regions of the detector. Of particular interest are superconducting tunnel junctions (STJs), fabricated on either a superconducting or an insulating substrate. X-ray detection occurs as a result of either direct photoabsorption, in one of the junction electrodes, or indirect photoabsorption, in the substrate.[1–9]

For both types of event, the required end result is that the photon energy is converted and transferred into excess populations of both quasiparticles and phonons within one of the STJ electrodes. The move from semi- to superconducting detectors is motivated by the fact that the magnitude of the energy gap of a conventional superconductor is of the order of meV, three orders of magnitude less than in current semiconductor devices, and such that the number of charge carriers produced as a result of photoabsorption will be three orders of magnitude greater, giving an improved resolving power. To be more explicit, the number of quasiparticles produced in a superconductor as a result of direct photoabsorption of a photon of energy E_0 is $N_0=E_0/\epsilon$, where ϵ is the energy required to create a quasiparticle. This number has an associated variance $\langle N_0\rangle^2=FN_0$, where F is the Fano factor.[10] The theoretical full width at half maximum (FWHM) resolution can therefore be written[6]

$$\Delta E_{\text{FWHM}}=2.355\sqrt{F\epsilon E_0},$$

which is of the order of eV for a 6 keV photon, compared with 120 eV for a conventional semiconductor detector.[11]

The spectral lines of interest in x-ray astronomy arise due to collisional excitations in a high temperature plasma ($10^6\rightarrow10^8$ K). At these temperatures, the principal elements radiate as heliumlike or hydrogenlike species. The K-shell line transitions have a variety of satellite transitions, and these cannot be resolved by semiconductor based detectors. For example, the He-like iron transitions, at 6.7 keV, require a resolution of around 10 eV, while the heliumlike oxygen lines, at 0.6 keV, require around 2 eV resolution. Such resolution requirements clearly favor the use of superconducting absorbers/detectors, and appropriately chosen materials/thickness for the absorber and junction can, in theory, fulfill these resolution requirements over the full energy range of interest.

An additional feature of superconductors that is of use in photon detection is the ratio of the energy gap to the Debye energy; in a superconductor the Debye energy is greater than the energy gap such that, during relaxation of the perturbed electron-phonon system, energy exchange between the two nonequilibrium populations can occur, i.e., phonon production does not necessarily constitute a major loss mechanism from the system.

The physics of the photoabsorption and relaxation processes is quite complex, and so only a summary is included here. Direct photoabsorption within a superconducting electrode results in the production of a high energy photoelectron (keV) that is rapidly absorbed, producing secondary electrons with energies of the order of eV. The atom relaxes after photoabsorption either by the emission of a fluorescent x-ray photon or Auger electrons. The probability of these relaxation routes is dependent on the material and the energy level responsible for the x-ray photoabsorption. Subsequent scattering of the secondary electrons finally results in an excess of quasiparticles of energy Δ, i.e., at the energy gap an excess, nonthermal population of phonons. The nonequilibrium populations are confined to a region that expands at a rate determined by the material, the material structure, and geometry.[1,12]

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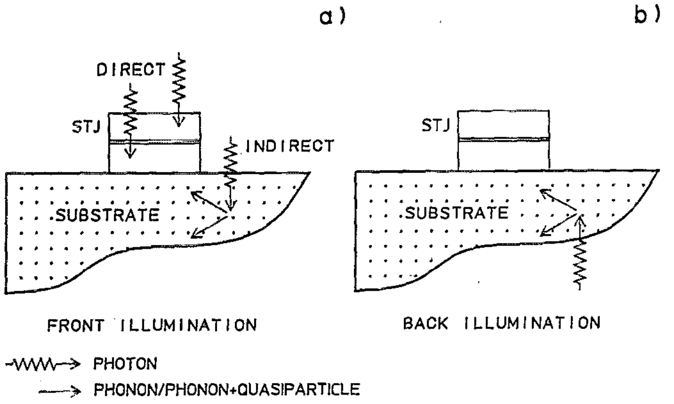

FIG. 1. The two modes of illumination (a) front and (b) back for an STJ detector. For both types of illumination, x-ray events occur in both STJ electrodes and the substrate at rates dependent upon the mass absorption coefficients and relative thicknesses of the substrate and junction materials. If the substrate is insulating, energy transfer to the junction is phonon mediated, whereas if the substrate is itself superconducting, energy transfer will rely upon both phonon and quasiparticle transport.

A similar final state in an electrode is also achieved in the case of indirect absorption: if the substrate is insulating, x-ray photons absorbed in the substrate produce an excess population of phonons that subsequently enter the junction, breaking Cooper pairs, and producing a nonequilibrium state. If the substrate is superconducting, the situation is more complex in that both phonons and quasiparticles will be produced in the initial photoabsorption; the nonequilibrium state in the junction is produced by both excess populations scattering into an electrode. Clearly, suitable combinations of insulator and superconductor are also possible for the absorbing regions. The thickness and composition of each region of the detector determines the number of direct and indirect events that will occur in the system. Figure 1 shows, schematically, some of the various possible detector/absorber configurations and illumination modes.

Direct absorption followed by relaxation of the excess quasiparticle population to the energy gap of an electrode is thought to take only an order of ns,[6,7] and the majority of models for the evolution of the nonequilibrium region of the electrode begin with the assumption that this initial relaxation process is complete.[1,9,13] Indirect events will clearly have quite different (and event location dependent) times associated with the production of an energy-gap excess population of quasiparticles in the electrodes: the excess population(s) produced in the substrate will take a finite time to get to the junction depending upon the reflection and transmission characteristics of the various absorber surfaces and interfaces, and also upon the substrate material and volume.

II. THE DETECTION PROCESS, LOSS MECHANISMS, AND SPECTRAL DEGRADATION

Subsequent relaxation of the gap-edge excess quasiparticle population in an electrode occurs by recombination of the quasiparticles to form Cooper pairs. During this relaxation process, the quasiparticles may tunnel across the insulating region into the neighboring film, giving rise to a detectable variation in the subgap current, so that the x-ray photon is detected. Any phonon of energy greater than or equal to the superconducting energy gap (2Δ), e.g., those produced by quasiparticle recombination processes, remains coupled to the quasiparticle population (via Cooper pair breaking), whereas any excess phonon of lower energy is decoupled and will eventually be lost from the system. Theoretical models indicate that this intrinsic loss mechanism will result in the energy required to produce a quasiparticle being equal to $\epsilon = \alpha\Delta$, rather than simply Δ. Simulations of the energy cascade in the superconductor have given estimates of α for niobium and tin to be 1.74 and 1.68, respectively.[6,14]

The smallest value of α yet found experimentally is 3.3, seen in niobium based junctions,[15] for a corresponding resolution of around 200 eV for an incident energy of 6 keV (Fe^{55}): the best resolutions obtained so far are of the order of tens of eV, dependent upon material, also for Fe^{55}, e.g. Refs. 4 and 16. Such results indicate that both serious loss mechanisms and additional sources of variance exist within the system. (Here, losses associated with fluorescent relaxation of the atom are ignored. This relaxation mode will in fact give rise to the "escape radiation" peak, e.g., at 3.7 keV in niobium.[17])

Mechanisms for loss of phonons of energy $\Omega \gg 2\Delta$ from within an electrode obviously exist: the thickness of the insulating region is an order of magnitude less than the phonon wavelength,[6] and as such is quite transparent to recombination phonons produced in either electrode. Similarly, the bottom electrode coupling results in extensive (and event location dependent) phonon loss from the junction to the substrate. Clearly, phonon loss from the top electrode to the substrate is (or can be made) negligible in comparison to that from the bottom since the junction thickness can be made greater than the phonon mean free path for Cooper pair breaking.[6,18] Phonon loss into the leads is also a possibility.[15]

Obvious routes for quasiparticle loss from an electrode are via diffusion of the excess quasiparticle population out of the barrier region, e.g., into the (superconducting) leads, or into regions of the lower electrode not covered by the insulating layer. In addition, photoabsorption in the leads can contribute significantly to the spectrum. Other mechanisms for quasiparticle loss have been suggested,[12] however, since the resolution generally obtained for a range of different materials and device configurations is still orders of magnitude worse than that predicted theoretically, it would appear that quasiparticle loss and the associated variance are still dominated by diffusion. Nevertheless, spatial variation in the superconducting properties of the film, e.g., Δ, as a result of both intrinsic, material inhomogeneity, and the experimental conditions will make important contributions to the variance by introducing an event location dependence into the original excess of quasiparticles N_0 and, hence, into the charge output.[19]

Indirect events rely upon energy transport from substrate to electrode in order to be registered and will therefore incur variances in addition to those already discussed.[20] First, the process itself is inefficient since the comparatively large volume of the substrate results in an incomplete energy transfer; some energy will always be transferred to the cold finger (and therefore lost from the system), even if this coupling is reduced.[6] Also, if the rate of energy transfer from substrate to junction is too low (e.g., for very large volume substrates) the nonequilibrium state produced in the electrode may not be sufficient to produce a detectable effect. Additionally, phonon transport in many typical insulating substrate materials has been shown to be highly nonisotropic,[21] and the phonon mean free path is extremely long,[22] producing a constant noise background and reducing the ability of the junction to resolve separate indirect events. So, for the case of indirect absorption, there is a significant dependence of the detected charge on the initial event location and the possibility of event confusion.

For the case of the substrate and junction that are well coupled acoustically, interference between direct and indirect events will occur: the high indirect event rate results in a continuous flux (although not constant as seen from the variance associated with these events) of energy from substrate to junction electrodes. This "background" contributes a further variance to the charge output produced by a direct event.

It is therefore clear that the substrate, both as source and sink, is playing a major role in spectral degradation. Elimination of these events, or a major improvement in the control of their associated variance, should improve the spectral resolution significantly.

Figure 2 shows a spectrum obtained experimentally for a niobium based STJ on a sapphire substrate. The area of the upper niobium electrode and barrier region is 144 μm^2, and the area of the lower electrode is 324 μm^2, resulting in a large region of the lower electrode, the "underlap" region, not being in contact with the barrier. The upper film thickness is 850 Å, and that of the lower film is 500 Å. The leads for both films of this device are 5 μm wide. The maximum charge output from this device is 30% of the charge generated by photoabsorption. A theoretical model including quasiparticle in- and out-diffusion to and from the leads and phonon transport to and from the substrate showed that the different regions of the device contribute to the spectrum, as indicated on Fig. 2.[15] The top film contribution quite clearly has a better resolution than the bottom film one, as would be expected from the previous discussion, and the majority of the "background" contributions are absorbed in the lower electrode. The noise tail, arising from the substrate, extends across the whole spectrum, and the junction leads and underlap regions[6] contribute a broad peak. Note that, since the junctions are generally so well matched acoustically to the substrate, any other vibrations in the system, other than those caused by photoabsorption, will also contribute to the spectrum.

III. DETECTOR OPTIMIZATION

The main goals of detector optimization are, therefore, to minimize the quasiparticle diffusion in and out of the film leads and to remove the substrate background contribution to direct events, in order to reduce the various contributions to the variance. In addition, the x-ray absorption efficiency of the detector must be maintained while simultaneously maintaining a high charge output.

While elimination of lead problems is relatively straightforward,[3] elimination or control of substrate contributions, both as an intrinsic noise source and as a heat sink for the junction, poses more of a problem.

A simple design for a direct absorption device that will be insensitive to all substrate contributions is shown in Fig. 3 and comprises a S'SIS system. Using the "semiconductor model" of a tunnel junction (Fig. 4), the functioning of

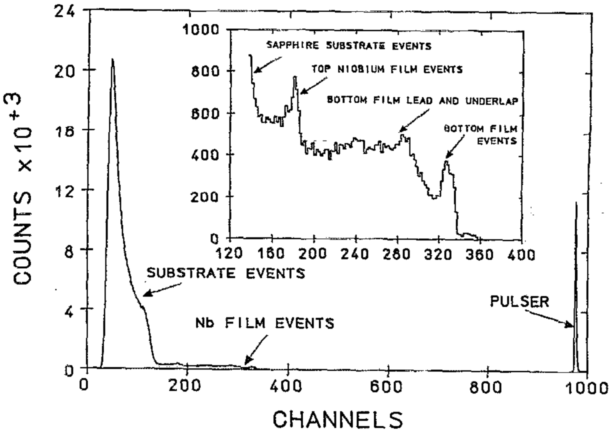

FIG. 2. The full spectrum of Fe^{55} x rays (6 keV) obtained from a Nb/Al/AlO$_x$/Nb junction with a highly transmissive barrier and, inset, the higher energy part of the spectrum arising from direct events. Different regions of the junction-substrate system contribute to the spectrum as indicated. From the inset it can be seen that the top electrode peak has a better resolution than that of the lower electrode since it is less strongly coupled to the substrate. A pulsar set at a charge output of 2×10^6 electrons is used to calibrate the system. The Mn K_α line from the bottom line is at 6.4×10^5 electrons. The equivalent FWHM of the pulsar line at the Mn K_α line energy is 40 eV. Although the Mn K_α and Mn K_β lines from the bottom film are resolved, the intrinsic variances in the detector dominate over the junction and system noise as measured by the pulsar.

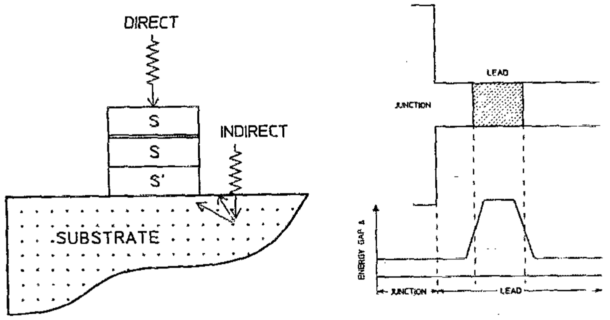

FIG. 3. Schematic of the basic proposed design for a device that decouples the substrate from the junction. The junction (SIS) is separated from the substrate by the layer S', where $\Delta_{S'} < \Delta_S$. The inset shows a schematic plan view of the junction lead with a region of higher energy gap superconductor inserted into it and the resulting pairing potential profile that prevents both in- and out-diffusion of quasiparticles.

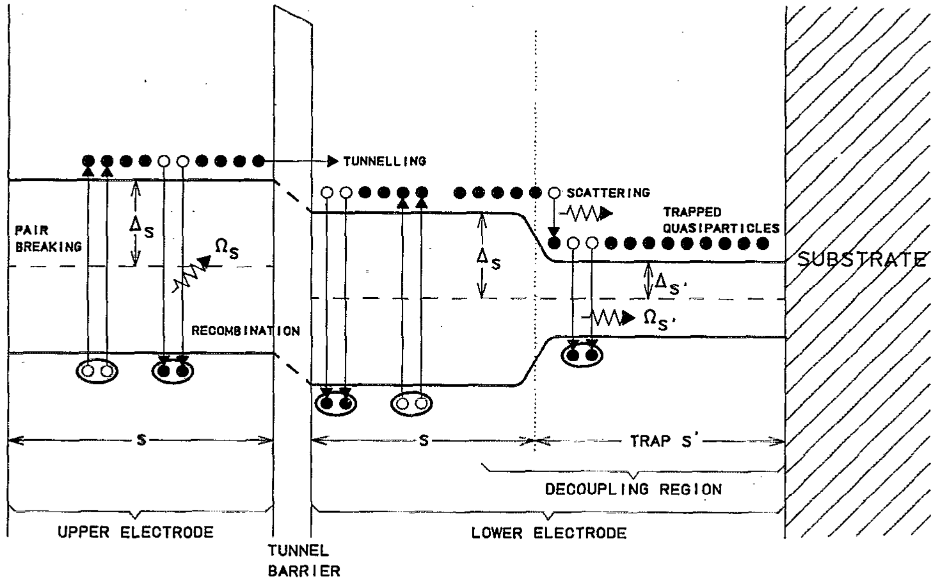

FIG. 4. Schematic of the proposed basic design and its mode of operation within the semiconductor representation. Photons absorbed in the upper electrode create an excess of quasiparticles, which then tunnel and are detected. Any photons stopped in the lower electrode bilayer will produce quasiparticles that are rapidly trapped within the trapping layer S′, far from the barrier. Phonons entering the junction from the substrate break Cooper pairs within the the decoupling region, producing trapped quasiparticles, and so do not contribute to the spectrum. Phonons produced via the recombination of trapped quasiparticles in the S′ region have too low an energy to break Cooper pairs in the S regions and will eventually be lost from the system.

this device can be understood as follows. The detection characteristics of the top film (S) will be unaltered by this configuration; however, the bottom bilayer film (S′S) contribution will be entirely removed.[2] The component of the bilayer in direct contact with the substrate (S′) is superconducting either due to its proximity to the upper component (S) or due to the operating temperature;[23] the only feature of importance is that the energy gap of this lower component is considerably less than that of the above, $\Delta_{S'} < \Delta_S$. This condition can be satisfied by an appropriate combination of materials of suitable thickness.[1,24]

Photoabsorption in the the lower energy gap region (S′) of the bilayer will produce excess quasiparticles that remain trapped in that region and also excess phonons that have too low an energy to couple to the Cooper pair sea of the neighboring film.[25] Photoabsorption in the higher energy gap component of the bilayer (S) will produce quasiparticles that are rapidly trapped in the low energy region[26] and a transient phonon population that will also rapidly disappear from the bilayer.[13] No contribution from the bottom electrode should therefore appear in the spectrum.

As previously outlined, the substrate acts as a source of phonons (and quasiparticles for the case of a superconducting substrate) for the junction. If the lower film of the bilayer S′ is thick enough, i.e., greater than the mean free path for Cooper pair breaking, then all such phonons will be absorbed within this region, producing trapped quasiparticles and phonons.

An additional feature of this device is that it eliminates another possible source of resolution degradation, back-tunnelling,[27] although the role of this mechanism in adding to the junction variance is unknown.

This approach should therefore provide a very clean spectral response from the detector, free from all contaminating effects of the substrate/bottom electrode coupling, and purely due to direct, top electrode events, without the need of resorting to experimentally difficult techniques such as substrate masking.[22] Any variance contribution for these events due to quasiparticle diffusion in and out of the leads can be eliminated, or at least severely reduced, by the use of a "pairing potential barrier" in a portion of the lead close to the point at which it contacts the upper electrode. Introduction of a small region of higher energy gap material into the lead, as shown in the inset of Fig. 3, will ensure that quasiparticles produced in the upper electrode remain there and will have a similar effect on any quasiparticles produced within the remainder of the lead. Previous approaches have used "pairing potential steps" to confine the quasiparticles within the electrodes,[3] using leads of a higher energy gap material than that of the junction. However, unless the x-ray photons are highly collimated onto the junction, such an approach does not prevent the nonequilibrium populations produced due to photoabsorption within the leads from diffusing into the electrodes.

Phonon loss from the top film across the junction barrier will still be a source of energy loss and therefore spectral degradation for this system, as will be (greatly reduced) phonon contamination from the bottom film events. However, this design allows for the experimental investigation of the intrinsic resolution of a superconducting film, in the absence of contamination from the substrate, such that it should be possible to investigate, for

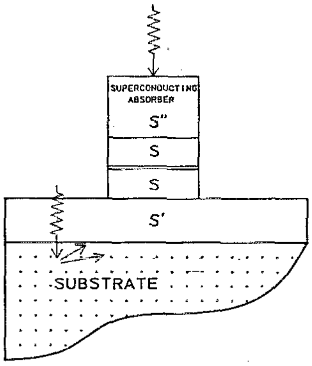

FIG. 5. The optimized device S"SISS' incorporates the use of an absorber, plus trap regions for the upper electrode. Photons absorbed in either region of the upper electrode create an excess of quasiparticles within the trap which then tunnel and are detected. The decoupling region may be extended to cover the whole substrate in order to change the quasiparticle trapping rates for the lower electrode.

example, the influence of variations in Δ, and the influence of the location of a direct event.

A requirement of x-ray detection systems, other than those outlined in the introduction, is good quantum efficiency. In the optimized device, the event rate can be increased by using a superconducting bilayer, S"S, for the upper electrode, where $\Delta_S < \Delta_{S''}$.[5] Photoabsorption occurring in the upper film of the bilayer S" produces quasiparticles that are subsequently trapped within S. Use of a trap has two advantages: it both increases the tunneling rate and amplifies the quasiparticle number, both of which enhance the output signal.[25] However, using such a bilayer region may result in further variance due to intrinsic variations in the amplification process. Photoabsorption will also occur in the trap S, and it is quite clear that this will not result in the same charge output as for an event in the absorber, since the quasiparticle production routes are quite different. Geometrical optimization of this bilayer should ensure that the thickness of the absorbing layer is large enough to provide a reasonable event rate, while the barrier area should be small enough to comply with the low capacitance requirements. In addition, the absorber volume should also remain small enough to provide a high enough rate of energy transfer to the trapping layer in order to obtain a detectable signal and to be able to deal with the photon count rate and prevent event confusion.

There are clearly a number of variations on this simple design, but most incorporate the basic building block of an SIS junction fabricated directly onto a quasiparticle/phonon trapping region, plus an upper, absorbing layer. For example, the detector could be of the configuration shown in Fig. 5, where the trapping layer S' extends over the whole substrate in order to improve the rate at which quasiparticles from the lower electrode S are trapped.

IV. SUMMARY

A simple design (that requires minimal modification to present fabrication techniques) for an STJ based x-ray detector, optimized for the purpose of investigating the intrinsic resolution of a superconducting film, has been presented. The new design eliminates noise contamination of the spectrum from substrate contributions through the use of a trapping layer grown directly onto the substrate. The quantum efficiency and charge throughput are increased by using a bilayer for the upper electrode: the upper component acts as an absorber and the lower as a trap. The spectrum resulting from this system is produced solely as a result of photoabsorption in the upper electrode, and additional degradation of this spectrum is reduced by the introduction of high energy gap regions into the leads.

Since the design removes or substantially reduces most sources of additional variance seen in the spectra, it is anticipated that such devices will lead further down the path towards Fano limited resolution.

ACKNOWLEDGMENTS

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