Lattice Damage in Superconducting Microcalorimeter Detectors

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***Abstract*—There is currently significant interest in using superconducting detectors for measurement of ion kinetic energies. Unprecedented resolution is possible with an order of magnitude improvement over semiconductors. Superconducting detectors are now able to probe the resolution limitations imposed by structural defects caused by incoming ions. Here we will calculate the expected resolution limits due to ion damage, as well as use the Monte Carlo simulation SRIM to compare results. Finally, comparison to on-going experiments will be made when possible.**

***Index Terms*—Lattice defects, microcalorimeter, Q spectroscopy, transition-edge sensor.**

I. Introduction

THERE is a long history of broad interest in the interaction of ions with bulk matter [1]–[4]. Most of this work has focused on interactions in Si and Ge since these have provided the highest resolution detectors in common use. These semiconductor detectors are fundamentally limited by Fano statistics to 8–10 keV full-width-at-half-maximum (FWHM) resolution for 5 MeV alpha particles [5]. Even at these resolutions, one begins to see broadening and pulse height defects due to energy stored in defect creation by incoming ions [6]. However, with energy resolutions as good as 0.7 keV FWHM at 5.5 MeV now possible by use of cryogenic calorimeter detectors, a new range of experiments probing ion interaction phenomena in a host of materials may now be possible [7]–[10]. In fact, the resolution of approximately 1 keV is not the fundamental limit of the detection technique. Based on signal-to-noise measurements and thermodynamic predictions, cryogenic detectors have shown intrinsic resolutions as good as 0.1 keV and the actual resolution is limited by defect creation [7].

Calculations of ion effects and their application to measurements in semiconductors were first done by Lindhard *et al.* [11]–[13]. Andersen realized the usefulness of these calculations for use with cryogenic detection techniques [14], [15]. In this paper we will briefly discuss the design of cryogenic detectors. Then we will use the calculations of Andersen, Lindhard *et al.*, and Haines *et al.*, as well as simulations with SRIM to compare to expected results from our detectors [16]. Some comparisons to experimental results will also be discussed.

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II. Cryogenic Microcalorimeters

Cryogenic calorimeters are made up of two basic elements: an absorber and a thermometer. In our group, we use superconducting transition-edge sensors, TES's, for thermometry. A TES is a thin film superconductor biased in its normal-to-superconducting transition so that small changes in temperature correspond to large changes in resistance. These have been discussed in detail elsewhere [7], [17]. Jang *et al.* have used metallic magnetic calorimeters as their thermometers, which rely on temperature dependent paramagnetism [10].

No matter the thermometer, one needs an absorber attached to the temperature sensor in order to convert an ion's kinetic energy into heat and a temperature change. The absorber is a bulk material that provides efficient absorption of ions while remaining within the heat capacity budget of the detector system.

There are two absorbing methods in use. The first is an external source method where an ion is emitted from a source external to the absorber. The source, however, is collocated with the detector in vacuum [7]. In this method, we have only had access to alpha particles in the 5 MeV range. Another method is termed embedded source, $4\pi-$spectroscopy, or Q–spectroscopy. In this technique, a radioactive source is embedded into the absorber so that alpha particles, gamma-rays, and daughter products are all absorbed essentially simultaneously giving rise to a single Q–peak [8]. The embedded source method has promise of simplifying source preparation and allows us to experiment with heavier ion bombardment. We have investigated tin and gold as absorbers in both detection schemes with ^{210}Po and ^{241}Am as sources of interest. Therefore, we will calculate expected lattice damage in these systems.

III. Lattice Damage

Andersen provides a nice treatment of the energy pathways within cryogenic calorimeters [14]. The main point for these detectors is that they only measure energy that is converted into heat. Thus, any energy that goes into mechanisms that do not result in an increase in heat on the measurement timescale of the detector will not be measured, or in the terminology of surface barrier detectors, contribute to pulse height defects.

When stopping ions, there are two main pathways for ion interaction with the bulk: electronic and nuclear. Both pathways thermalize much faster than the bandwidth of the detector. The electronic interactions are inelastic energy loss to the target electrons. This pathway can lead to excited electrons as well as energy lost to emitted photons. Since the calorimeters use bulk targets, however, all of the processes stemming from the electronic branch will thermalize into heat.

The nuclear pathway is comprised of scattering with atomic nuclei that results in atomic motion in the absorber lattice. The atomic motion can thermalize and be measured, but some motion will result in structural defects, or lattice damage, in the absorber. Since we are working at cryogenic temperatures, these defects will be stable and any energy stored in these defects will be lost from our measurement. The key parameters controlling defect production are the amount energy going into atomic motion, ν, the displacement energy, $E_{\mathrm{d,eff}}$, which is the energy necessary to move an atom from its lattice location, and the Frenkel storage energy, Q, which is the energy stored when a displaced atom rests in an interstitial site in the lattice. Energy loss does not degrade resolution but does affect signal-to-noise. Fluctuations in the energy loss will, however, degrade resolution by adding in quadrature to the thermodynamic resolution and is what we will calculate presently.

We will adapt published calculations for lattice damage to the detector systems with which we are working. In particular, we are interested in the decays of ^{210}Po, since it provides a single peak for characterization, and ^{241}Am which has been a convenient source used for Q–spectroscopy measurements. We will also compare these calculations to SRIM Monte Carlo simulations and experimental results.

IV. Calculations

A. ^{210}Po

The decays we are interested in here result in two main products that affect resolution: the alpha particle and the daughter product. For ^{210}Po, we are interested in a 5304.38 keV alpha particle and a 103.08 keV daughter ^{206}Pb. The first step in calculating the lattice damage from an incoming ion is calculating how much energy goes into atomic movement. We will start with the alpha particle.

Alpha particles are very light ions with large incoming energy. Thus, the nuclear scattering cross section is very low and little energy goes into atomic movement. Lindhard found that the energy in atomic movement, ν, from alpha particles at high energy had very little dependence on energy and bulk material yielding approximately 12 keV [13]. Lindhard calculates collisions in two groups separated by energy T^*. Since the energy going into atomic movement will form a Gaussian, T^* is chosen to be the width of the Gaussian, $\Delta\nu$. Energies far above T^* will form a high energy tail but not contribute to the Gaussian width. Thus, using Lindhard's (5) from [13], multiplying by the correction for incoming energy in the same reference, setting T^* equal to $\Delta\nu$, and solving we get the expected width of energy in atomic movement of,

$$\Delta\nu = \lambda + \sqrt{\lambda^2 - \chi^2}, \tag{1}$$

where

$$\lambda = \frac{1}{2}\left(2\chi + \frac{4}{9}\frac{\chi^2}{\gamma E}\right) \tag{2}$$

$$\chi = \left(\frac{Z_1^{\frac{5}{6}} Z_2 Z A_1^2}{A_2^{\frac{1}{2}}(A_1 + A_2)} \frac{e^2}{4\pi\epsilon_0}\sqrt{\frac{M_p v_0^2}{2}}\right)^{\frac{2}{5}} \tag{3}$$

$$\gamma = \frac{4A_1A_2}{(A_1 + A_2)^2} \tag{4}$$

$$\nu_0 = \frac{1}{4\pi\epsilon_0}\left(\frac{e^2}{\hbar}\right). \tag{5}$$

Here, E is the incoming alpha particle energy, Z and A are atomic number and mass respectively with the subscript 1 denoting the ion and subscript 2 the target, e is the electron charge, ϵ_0 is the permittivity of free space, a_0 is the Bohr radius, and M_p is the proton mass. Thus, the FWHM Gaussian width of the energy going into atomic movement for the ^{210}Po alpha particle into a Sn absorber is $2.355\Delta\nu$ which is 6.2 keV. The same decay into Au yields a fluctuation of 6.7 keV.

At this point, we use Andersen's equation based on collision cascade theory to determine the amount of energy stored in defects [14]. The fluctuation in the number of defects created, δn, will be

$$\delta n = \frac{0.42(\delta\nu)}{E_{\mathrm{d,eff}}}, \tag{6}$$

where $E_{\mathrm{d,eff}}$ is the effective displacement energy of the absorber. The same equation for average energy lost to a target yields the expected pulse height defect. For Sn, the effective displacement energy is 28 eV [18]. We then multiply (6) by the Frenkel storage energy, Q, to ascertain the contribution to the detector resolution, δE. The Frenkel energy is an unknown quantity for most metals, but a reasonable approximation to begin with is 4 eV [18]. which would give a broadening to the FWHM detector resolution of 372 eV and an average energy loss of 700 eV. For Au, the displacement energy is 43 eV, so that for the 4 eV Frenkel energy, one expects a broadening of 262 eV and loss of 500 eV.

For embedded sources, we must account for the damage from daughter products, which for ^{210}Po is ^{206}Pb. It would also be interesting to see if the ^{206}Pb pulses from external ^{210}Po show the expected damage broadening, but these measurement have not been done yet.

For this calculation, we use the estimates of Haines *et al.*, who used a second order scattering calculation based on Linhard's Thomas-Fermi scattering cross section to calculate energy loss and fluctuation in energy loss due to heavy ions [6], [11]. We will use the numerical calculations of Haines that result in Figs. 2 and 3 in [6]. Lindhard defines a unitless energy, ϵ, based on the system under study as [11]

$$\epsilon = \frac{E}{k_E}, \tag{7}$$

where

$$k_E = \frac{e^2}{4\pi\epsilon_0}\frac{Z_1 Z_2 (A_1 + A_2)}{a A_2}. \tag{8}$$

TABLE I
COMPILATION OF FWHM RESOLUTION FROM DAMAGE STATISTICS

Particle	Calculations (eV)	SRIM (eV)	Experiment (eV)
^{210}Po alpha in Sn	372	300	900 [7]
^{210}Po alpha in Au	262	260	1700 [8]
^{210}Po Q in Sn	6400	1100	–
^{210}Po Q in Au	3900	580	2600 [8]
^{241}Am alpha in Sn	416	280	–
^{241}Am alpha in Au	263	223	–
^{241}Am Q in Sn	5900	1400	–
^{241}Am Q in Au	3600	770	3000 [8]

The variable, a, is the approximate length where Coulombic screening is important and is

$$a = \frac{0.8853 a_0}{\sqrt{Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}}}}. \tag{9}$$

Once we have defined the unitless energy, the plots in [6] yield dimensionless energy loss, $\overline{\Delta\epsilon}$, and the FWHM fluctuation in the energy loss, $\delta\epsilon$. We may then convert back to energy loss and fluctuations for a particular system by

$$\nu = k_E \overline{\Delta\epsilon} \tag{10}$$

$$\delta\nu = \gamma^{\frac{1}{2}} k_E \delta\epsilon. \tag{11}$$

The variables are previously defined for (1).

For the ^{206}Pb into Sn, $\epsilon = 0.05$, yielding $\overline{\Delta\epsilon} = 0.05$, so all energy goes into atomic motion at this energy scale. This translates into a loss of energy from the detector signal due to stored atomic displacements of 6.4 keV. Also, $\delta\epsilon = 0.05$, yielding $\delta\nu = 95$ keV and a FWHM contribution to a spectrum from (6) of 6.4 keV. Using Au as the absorber, we get $\epsilon = 0.04$, a FWHM fluctuation of 3.9 keV and loss of 4.0 keV.

B. ^{241}Am

We have also conducted experiments with the isotope ^{241}Am so calculations pertaining to Au and Sn as absorbers are interesting. We need to calculate the effects of a 5485.56 keV alpha particle from ^{241}Am and a 92.7 keV recoiling ^{237}Np.

Using (1) and (6) with Sn as the absorber, we see a fluctuation contribution from the alpha particle of 416 eV. With Au as the absorber, the fluctuation contribution from the alpha particle is 263 eV. Using the Haines calculation for heavy ions the fluctuation predictions for the ^{237}Np into Sn and Au are 5.9 keV and 3.6 keV respectively. The resolution predictions are summarized in Table I and the average energy losses are shown in Table II.

V. SRIM SIMULATIONS

We have also modeled the expected damage spectra using the ubiquitous SRIM Monte Carlo simulation package [16]. The same parameters as used in the calculations, namely ion energy, mass, displacement energy of the absorber, and Frenkel storage energies are used for the simulation. The SRIM code calculated the number of displacements in the lattice for every ion and resulting cascades. By summing the displacement for every ion, we create a spectrum of lattice damage. We then multiply the displacement by the Frenkel storage energy and subtract this spectrum from the expected monoenergetic value. We then fit the spectrum using a convolution of a Gaussian with an exponential to account for straggling [7]. The results of the simulations are shown in the table in the next section. The alpha particle from a given decay and the resulting nucleus are each modeled. Then the spectra are added ion by ion to yield the expected Q-spectra.

TABLE II
AVERAGE ENERGY FROM ION LOST TO LATTICE DAMAGE

Particle	Calculations (eV)	SRIM (eV)
^{210}Po alpha in Sn	700	480
^{210}Po alpha in Au	500	470
^{210}Po Q in Sn	6200	7760
^{210}Po Q in Au	4000	6100
^{241}Am alpha in Sn	700	450
^{241}Am alpha in Au	500	430
^{241}Am Q in Sn	5500	10200
^{241}Am Q in Au	3600	8720

VI. SUMMARY OF RESULTS AND COMPARISON TO EXPERIMENT

Tables I and II show a summary of the results discussed in this paper. Experimental data, when known, is also shown for comparison. Alpha refers to calculations and measurement of only the alpha particle emission from a given isotope. The Q value refers to the sum in quadrature of the alpha particle damage fluctuations and the daughter product. However, since the daughter product dominates damage production, the Q value is equivalent to the heavy ion calculation. The first point taken from this analysis is that the Lindhard calculations for alpha particle damage resolution degradation agree with the low SRIM values. However, the calculations for heavy ions come much closer to the results seen in experiment. A second point of the results is that the SRIM code consistently underestimates damage fluctuations for both alpha particles and heavier ions. It would appear that alpha particle simulations are a factor of three below expected values, an a factor of six low for Q spectroscopy values.

VII. CONCLUSION

Microcalorimeter detectors provide a new level of energy resolution for the study of ion impacts. For the first time, lattice damage is the limiting factor for resolution. This may open up directions for the study of basic ion interactions with matter. We have compared a small set of measurements with classical scattering calculations and Monte Carlo simulation. We observe areas of agreement and disagreement both between the calculation methods used and between these and the experimental results. Data from microcalorimeters may allow rigorous evaluation of scattering theories resulting in improved theoretical capability. Once a suitable theory is established, microcalorimeter data may allow the determination of parameters such as the Frenkel energy in a wide range of previously unmeasured materials.

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