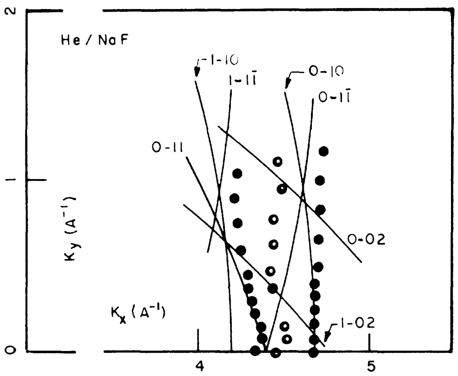

FIG. 2. Wave-vector components for minima of curves in Fig. 1. Solid lines are circles corresponding to zeroth-order energy levels according to Eq. (5). Dot size indicates estimated error.

son calculated a splitting of about 6° for LiF, based on a model potential with several empirically fitted parameters. Our experimental results on NaF (Fig. 1) show splittings of the same order of magnitude. However, rather than a simple crossing of two otherwise isolated levels, we see that the situation is complicated by the presence of numerous other zeroth-order levels in the same vicinity. The observed positions of the minima suggest mixing of the following pairs of zeroth-order states: [0-1, 0] and [0-1, $\bar{1}$], [0-1, 1] and [1-1, 0], and [1-1, $\bar{1}$] and [1-1, 0] in the notation [j-m, n]. These pairs are all connected by reciprocal-lattice vectors of the (0, 1) type.

On the other hand, the [0-0, 2] level has no discernible effect, as it is connected with the others by longer reciprocal-lattice vectors. This is actually the far more prevalent situation. As further examples, the [j-0, 1] and [j-1, 0] pairs cross at $\varphi = 45°$ with no discernible perturbations, as do the [j-0, 1] and [j-0, $\bar{1}$] pairs at $\varphi = 0°$. In fact, such crossings are of great assistance in identifying the minima and determining the energy values needed for the radii of the circles drawn in Fig. 2.

Thanks are due to the National Science Foundation and to the Applied Research Laboratory of The Pennsylvania State University for their support of this work, and to Professor Eric Thompson for preprints and discussions of his work in advance of publication.

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*Work supported by National Science Foundation under Grant No. DMR75-16603 and by the Applied Research Laboratory of The Pennsylvania State University.

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Evidence for Temperature Dependence of Positron Trapping Rate in Plastically Deformed Copper

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(Received 12 August 1976)

Doppler-broadending studies have been conducted on the γ rays following annihilation of positrons in plastically deformed copper samples. Evidence for a temperature dependence of the trapping rate comes from the observation that in the sample investigated the fraction of positrons trapped varied by 30% in the range 6–77 K.

This Letter reports a new discovery concerning the trapping of positrons by defects in copper at very low temperatures. Earlier measurements in the range 77 to 270 K by MacKenzie *et al.*[1] on nickel, and Rice-Evans and Hlaing[2] on copper had given no indication of the observed effect, viz., that the rate of trapping declines with diminishing temperatures.

Positron annihilation has become an important probe in the study of metals.[3-5] It was Berko and Erskine[6] who discovered that plastically deformed metals trapped positrons prior to their annihilation; and it is now known that many defects such as monovacancies, dislocations, and voids can trap positrons, and that the properties of the annihilation photons are accordingly modified. A matter of particular theoretical interest is the temperature dependence of the trapp rate.[7-11] In this work the trapping by dislocations in copper has been investigated in the temperature range 6 to 77 K.

The shape of the 511-keV annihilation line in copper has been studied with a high-resolution (1.15 keV for the 514-keV ^{85}Sr line) germanium γ-ray detector. It is assumed that positrons quickly slow down to thermal energies on entering the copper and that the resultant momentum of the e^+e^- pair causes a Doppler-broadening of the annihilation line.

Essentially, the participating electrons fall into two classes: core and conduction electrons. To a considerable extent these yield the well-known Gaussian and (narrower) parabolic components of the annihilation line. If the positron is trapped in a defect, the probability of annihilation with a conduction electron is enhanced, and this can be observed by noting the change in the normalized height of the line. Of course, while being useful in defect studies, this simplified picture actually hides the whole truth concerning the components of the annihilation line (Ref. 4).

To study the temperature dependence of trapping 1-mm-thick samples of 99.999% pure copper (from Johnson Matthey) were plastically deformed at room temperature to produce fixed concentrations of defects—dislocations.[12] The deformed samples were allowed to age for several weeks prior to measurement, to allow monovacancies to anneal out, and then etched. Two specimens were measured: (A) One specimen with a defect concentration produced by hammering the specimen to reduce its thickness by about 10% and (B) an undeformed annealed sample.

The ^{64}Cu positron source was an irradiated 5-μm-thick copper foil; and this was sandwiched between the copper samples. The specimen was inserted in a vacuum cryostat immersed in liquid helium; and temperatures up to 77 K measured with a thermocouple were obtained by employing an Oxford temperature controller. Because of the 12.9-h source half-life, the distance between the detector and the specimen was adjusted every 90 min, so that the detector should operate continuously at 3000 Hz.

A linear representation of the proportion of annihilations occurring in the trapped state may be given by the F parameter, which in our case has been defined as the number of counts in the central 21 channels of the line normalized to the total peak area, which corresponded to about 40% of the total. Drifts in the line position of up to 0.02% were observed, and allowance was made for this in the calculation of F by moving the limits of the central region.

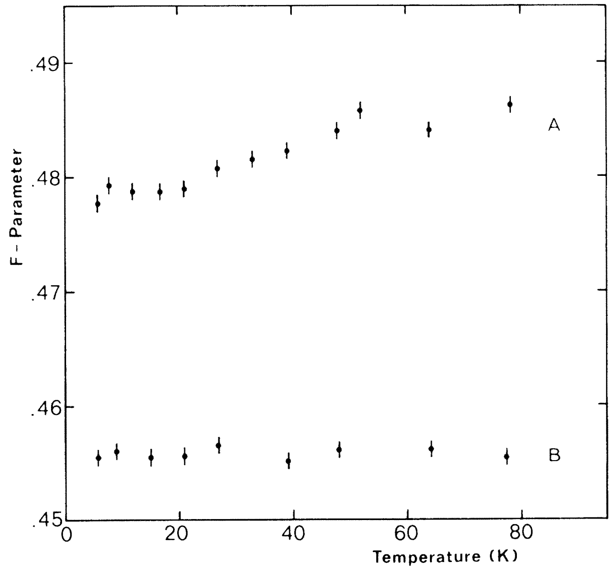

FIG. 1. The variation of the F parameter over the temperature range 0–77 K. (A) A moderately deformed sample; (B) an annealed sample.

In Fig. 1, the variation of the F parameter with temperature is shown for the two specimens. Each point corresponds to a line containing 600 000 counts. The lower set of points indicates the annealed sample (F_f); the top set, the case of the deformed sample (F).

The definition of F allows one to write for cases of intermediate deformation

$$F(T) = PF_t + (1-P)F_f, \qquad (1)$$

where F_t corresponds to saturation trapping and where P, the fraction of positrons trapped at annihilation, is given by

$$P = \frac{\mu(T)C/\lambda_f}{1+\mu(T)C/\lambda_f}, \qquad (2)$$

where $\mu(T)$ is the trapping rate, C the concentration of defects (considered constant),[12] and $1/\lambda_f$ the positron lifetime.

Curve A in Fig. 1 actually represents one of three similar runs on a deformed sample at these low temperatures. Curve B shows that there is no temperature variation in F for the annealed sample. Figure 2 is shown for compar-

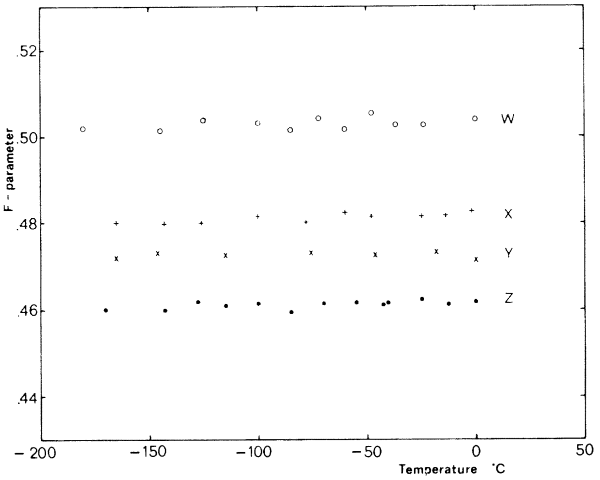

FIG. 2. The variation of the F parameter for the deformed (W, X, Y) and annealed (Z) specimens in the temperature range 100 to 270 K. The values of F here and in Fig. 1 are not strictly comparable because of instrumental modifications.

ison.[2] The annealed sample (Z), the grossly deformed sample causing saturation trapping (W), and two moderately deformed samples (X and Y) exhibit essentially no temperature dependence in the range 100 to 270 K. Sample (A), though not identical with (X), was produced in the same manner; and hence one can assume the flat nature of the curve for (X) in the region 77 to 273 K will also be true for (A).

From curve A we see that below about 60 K the assumed plateau ceases and it is clear that F is influenced by the temperature of the specimen. With an appropriate reconciliation of the F parameters in Fig. 1 and 2 (the data having been taken with different crystals) and taking the sample (W) to represent the case of 100% trapping, the data of Fig. 1 suggest that the fraction of positrons trapped rises from $(56\pm2)\%$ at 6 K to $(73\pm3)\%$ at 77 K (i.e., a variation of about 30%).

The decline in F at low temperatures is difficult to explain. It is inconceivable that at the lower temperatures the concentration of traps should diminish. Neither can we expect the probability of positron escape from a trap to be increased. From the behavior of the annealed specimen (Fig. 1), we see that F_f remains constant; and we can see no reason why the parameter F_t should decrease. Hence from Eqs. (1) and (2) it is reasonable to conclude that it is the trapping rate μ that diminishes.

A recent theoretical discussion has been that of Frank and Seeger.[13,14] They considered both diffusive motion of the positron towards the trap, and the overcoming of a barrier prior to trapping, and wrote

$$\mu=\frac{4\pi r_0}{\Omega_A}\left(\frac{1}{D_+}+\frac{1}{k_0 r_0 \Delta_0}\right)^{-1},$$

where Ω_A is the atomic volume, r_0 the capture radius, Δr_0 the width of the barrier, and k_0 the rate constant for capture by the trap.

This equation may be invoked to account for the lack of temperature dependence seen in the region 77 to 270 K. In this case, the capture term might predominate over the diffusion term. Hodges[8] has treated the trap as a potential well and has found the resultant trapping rate to be independent of temperature. Bergersen and Taylor[15] support this view.

A possible explanation for, or contribution to, the observed decline in F may lie in the diffusion term. Much work has been done on the complicated question of diffusion. Brandt[11] has combined the effects of positron scattering on electrons, phonons, and crystal imperfections to give (respectively) for the diffusion coefficient:

$$D_+=\frac{\hbar}{\pi m_+}\left[2.5\times10^{-5} r_s^{2}\left(\frac{T_+}{300\text{ K}}\right)+5\times10^{-2}\left(\frac{T_+}{300\text{ K}}\right)^{1/2}+BC_{sc}\left(\frac{300\text{ K}}{T_+}\right)^{b}\right]^{-1}.$$

Here T_+ is the effective positron temperature and C_{sc} is the concentration of scattering centers. The first two terms would give a temperature dependence of F in a direction opposite to that observed, but the third term might be responsible. The constants B and b depend on the properties of the crystal imperfections, with $\frac{1}{2}\leqslant b\leqslant\frac{3}{2}$. In a deformed sample, there will be a multitude of imperfections. Brandt[11] suggests the first two terms are usually small compared to the third, although in the expression this actually depends on the values assumed for B, b, and C_{sc}. It must be added that both Connors and West[16] and Bergerson and Pajanne[9] have considered models that result in $\mu(T)\propto T^{1/2}$.

An important question is whether positrons are thermalized before annihilation at these low temperatures. Contrary to earlier opinion, Kubica and Stewart[17] have recently employed high-resolution angular correlation apparatus to find that positrons approach thermal energies at liquid-helium temperatures (e.g., 10 K in magnesium); and thus one may reasonably assume that they will do so in copper.

Another factor that might help explain the data could be that the rate of capture depends on temperature; and in principle one might use the Seeger expression with a variable capture term. A simpler approach would be to take a classical model of a trap, i.e., a potential well surrounded by a slight barrier, with the positrons finding increasing difficulty in overcoming the barrier, prior to trapping, as their temperatures were reduced. Such a model would lead to barrier heights of the order of meV, but estimates would have to be made of the relative times for rethermalization, trap encounters, and annihilation. However in view of the many uncertainties it is hardly sensible to speculate further; the new effect calls for further detailed experiments with good statistical precision and known concentrations of defects.

We are pleased to thank Professor E. R. Dobbs for his interest; Dr. M. J. Lea and Dr. D. Almond, for their cryogenic advice; and A. O. T. Lemottee, J. Sales, F. Grimes, A. King, B. Pashley, and Mildred Piper, for their assistance; and the Science Research Council, for their financial support.

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Contributions to Localization in the Silicon Inversion Layer from States in the Gap in SiO_x†

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(Received 13 May 1976; revised manuscript received 26 July 1976)

Recent experiments on silicon inversion layers in the activated conductivity regime have shown a variety of electronic behaviors which are in marked disagreement with the predictions of Mott-Anderson localization, which is due to random static-potential fluctuations. It is argued here that there is an additional mechanism causing electron localization which involves electron-pair states in the energy gap of the disordered oxide. It is shown that by including this mechanism it is possible to account for a variety of these electronic properties including the dependence of the mobility edge on electron density.

The quasi–two-dimensional electron gas formed by inversion layers in metal-oxide-semiconductor structures has been the subject of much study.[1] It has been suggested that at low surface electron densities n_s ($\lesssim 10^{12}$ cm^{-2}) the electrons become localized in the Mott-Anderson sense,[2] and thermally activated conductivity in this regime has been observed. Important features observed experimentally in this regime, however, are at variance with the results of the Mott[3] theory of localization. Such examples include a mobility edge which is a strong function of n_s for devices with low fixed oxide charge Q_{ss},[4] large variations in the supposedly constant "minimum metallic conductivity,"[5] and a decrease in the activation energy with increased substrate bias.[6,7] Furthermore, well-defined magnetoconductance oscillations[4] and Hall effect,[8] and anomalous fre-