

This paper by Bickford and Kanazawa set a landmark standard for measurement of the conductivity of highly anisotropic materials. Its appearance in late 1975 corrected several serious errors that had been published at the time...one by a future Nobel Laureate!

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ELECTRICAL CONTACTS ON ORGANIC CRYSTALS: TTF-TCNQ

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Abstract—Room temperature plots of the electrical potential measured on the surfaces of TTF-TCNQ crystals which carry current are presented. It is shown that silver paint contacts behave electrically as though thin resistive layers (≤ 20 mhos/mm² conductance) were inserted between the crystal and the current-injecting electrodes. The contact resistance is microscopically nonuniform, and can lead to erroneous results in 4-probe conductivity measurements. By measurement and calculation (using the method of image charges) it is demonstrated that measurement techniques which introduce nonuniform current densities into highly anisotropic crystals are subject to error unless the contacts are kept very small. The principal conductivities of TTF-TCNQ at room temperature were found to be: $\sigma_b = 440 \pm 15$, $\sigma_c \approx 13$, $\sigma_a = 1.30 \pm 0.05 \Omega^{-1} \text{cm}^{-1}$, independent of contact effects.

INTRODUCTION

Increased attention recently has been focused on the influence of contacts on conductivity measurements of highly anisotropic conducting crystals of TTF-TCNQ. These studies[1-4] have concerned themselves almost exclusively with the difficulties arising from the inexact geometric placement of the current-injecting contacts. The current distribution and therefore the apparent conductivity are extremely sensitive to contact geometry in anisotropic crystals. It is generally felt that these difficulties can be resolved by using the measurement technique due to Montgomery[5].

During the course of our conductivity study it quickly became apparent that a factor in addition to the geometrical placement of the contacts was important: namely, the microstructure of the silver paint/crystal interface. Our subsequent investigations of contact behavior have yielded results which we believe will be of general usefulness to those involved in the measurement of electrical conductivity in anisotropic media. They are the subject of this paper.

The crystals used in our experiments were grown by carefully controlled diffusion of the donor and acceptor at room temperature in a conventional U-tube. The starting materials were at least 99.9% pure. Polarized optical microscopy showed that the crystals have the usual platelet habit; viz. with the longest axis along the highly conducting *b*-direction. Only striation- and step-free crystals showing well-developed faces were used in our experiments.

While a variety of electrode materials (metals and alloys) and electroding techniques (evaporating, electroplating, amalgamating) were used at various times during this study, all of the work reported here deals with silver paint contacts. We found the contact resistance of the silver paint to be at least as low as the values we obtained

with metal and alloy films. Therefore we could see no reason to ignore the enormous advantage offered by the convenience in applying and handling silver paint. Two different formulations† were used. There was no discernible difference in their properties. The room temperature resistivity of the silver paint alone (thoroughly air dried) was measured to be 6×10^{-5} ohm cm.

EXPERIMENT

Our basic technique was similar to that employed by Zosel *et al.*[6] during their investigation of other anisotropic TCNQ salts. A carefully selected crystal of TTF-TCNQ was mounted within the field of view of a binocular microscope. Two current-injecting silver paint electrodes were applied to the ends of the crystal and then attached to gold wire leads. One of the electrodes was grounded, while the other was attached to a constant current source which supplied a d.c. current of 100 μA .‡ By means of a movable third contact, the potential at any point on the crystal surface could be determined. This third contact consisted of a small-diameter (12.5-50 μm) gold wire which was positioned by means of a micromanipulator. Even though this potential probe carried no current, it sometimes was difficult to make it establish good electrical contact with the crystal. One technique which tended to improve the contact was to melt the end of the wire to a ball of diameter about twice the wire's diameter, and then to coat the ball with mercury. We found that the relatively large thermoelectric effect[7] in TTF-TCNQ can result in spurious potentials of the same order of magnitude as those being measured. Therefore, care had to be taken to insure that there were no thermal gradients in the sample (as from a microscope lamp). The invariance of the magnitude of the potentials to reversal of the current direction was used as an indication of the absence of thermal gradients.

The current-voltage relationships of this system were found to be linear over several decades: at least up to values of current two orders of magnitude larger than the 100 μA used in most of the measurements. From this fact one can conclude that whatever contributes to the

†DuPont No. 7941 and No. 4929, with 2-butoxyethylacetate solvent.

‡It was established by current pulse measurements that this current caused no thermal effect.

current-voltage relationship must itself have a linear characteristic. In particular, the bulk electrical behavior of TTF-TCNQ must be linear, and the contact interface with the silver paint can be characterized by an ohmic contact resistance.

In our early studies the potential distribution was not examined over the entire crystal surface. Only the variation of potential along a line parallel to the current-carrying direction was determined. A particularly good example of such a study is shown in Fig. 1. Here the current is flowing parallel to the *b*-axis. In principle, at least, the current density is uniform throughout the sample. Figure 1 shows evidence for three identifiable resistances.† First, there is a small but finite resistance due to the silver paint itself (points 1-2 and 15-16). Second, there is the interfacial contact resistance between the silver paint and the bulk crystal (points 2-3 and 14-15). This interfacial region was found to be very thin. It was thinner than our resolving power of 10 μm. Finally, there is the bulk resistance of the crystal itself (points 3-14). The contacts had been made to cover the entire end surfaces of the crystal, in order to guard against possible current variations in the *c**-direction (normal to the plane of Fig. 1). Therefore, the slope of the curve in this linear region gives the bulk conductivity independent of any contact effects.

As our techniques became more refined we began to obtain the entire potential topography of a given surface. By plotting equipotential lines across the crystal face it was possible to monitor the uniformity of the current flowing through the sample. In the case of a rectangular crystal with opposite ends completely covered by silver paint contacts, the equipotential lines should be parallel straight lines perpendicular to the direction of current flow. Figure 2 represents four of many attempts to obtain

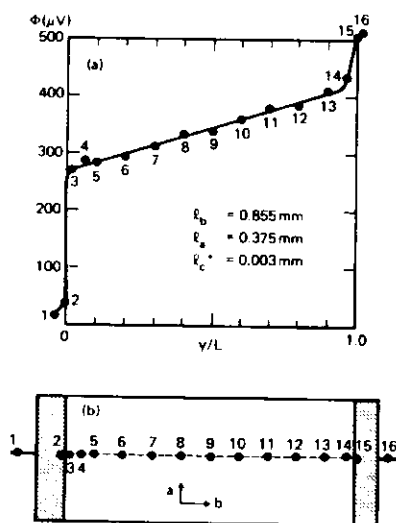


Fig. 1. (a) Potential profile of TTF-TCNQ crystal along its *b*-axis. (b) View of *a*-*b* crystal plane showing location of measurement points.

†The resistance of any region is given by the ratio of the potential drop across that region to the current through it.

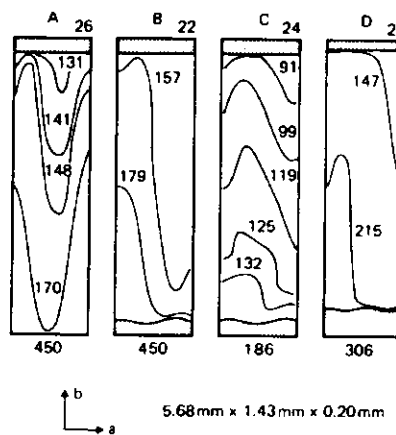


Fig. 2. Measured equipotential lines on a specimen of TTF-TCNQ carrying "uniform" current in the *b*-direction. Diagrams A, B, C and D represent four different sets of silver paint contacts. Numbers give the potential in microvolts.

this ideal pattern on a sample of exceptionally fine crystal habit. After each unsatisfactory result one of the contacts was repainted in an effort to achieve a uniform contact of low contact resistance. Figure 2(c) represents the closest approach to the ideal curves which we were able to achieve using this crystal.

RESULTS AND DISCUSSION

At first sight there would seem to be a basic incompatibility between the results of Fig. 1 and those of Fig. 2. However, this is not the case. From Fig. 2 one can obtain a number of different curves of the Fig. 1 type by drawing vertical lines at different lateral positions on the crystal. If one plots potential vs distance along those lines, the result still can be interpreted in terms of straight lines of generally the same slope. However, usually there will be much more scatter among the individual points than is seen in Fig. 1. This scatter increases the probability that the slope (and thereby the resistivity) will be determined inaccurately. Although most of the lines will have roughly the same slope, they will have different intercepts at the ends. In other words, the effective interfacial contact resistances, as defined in Fig. 1, will be different.

The "instability" of the equipotential lines which is illustrated in Fig. 2 can be the result of only one of two things: either the crystal suffers from significant internal inhomogeneities, or the contact interfaces are nonuniform and irreproducible. The former possibility is most unlikely, since the different equipotential patterns retain no common feature. The fact that the patterns change when the contacts are re-applied indicates that the contacts themselves are the source of the problem.

There exists in the literature indirect evidence for the irreproducibility of contacts. Cohen *et al.*[1] reported that only those TTF-TCNQ crystals which showed an overall resistance of 10 Ω or less were used in their experiments. This implies that the contact resistance varied widely among the crystals. Since all of the contacts illustrated in Fig. 2 yielded resistances smaller than 10 Ω, it is obvious that a low overall resistance is no guarantee that the current and potential patterns will be well-behaved.

We set inhomogeneous four-probe distribution contacts, before expected, altered by the equipotential potential making good area.

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Fig. 3. Potential (upper) contact

†Cutting was shape (and also the *b*-axis) were the crystal is not concerned

‡This same much lower cor

We set out to obtain more direct evidence of contact inhomogeneities. In one set of experiments using the four-probe technique, we obtained the equipotential distribution of a crystal, with its current-carrying contacts, before and after potential contacts were applied. As expected, the shapes of the equipotential lines were altered by the presence of the new contacts. In one case the equipotential lines appeared to run under a part of the potential contact, indicating that the silver paint was not making good electrical contact with the crystal in that area.

A more conclusive experiment is illustrated in Fig. 3. Both ends of another fine crystal were cut off, using a very sharp razor blade.† One end was completely covered with silver paint, carefully applied to avoid overlapping the other faces. This created a plane contact. A 12 μm gold wire coated with a very thin layer of silver paint was attached vertically to the opposite end. This approximated a line contact, so that the crystal had a line-plane electrode configuration. Figure 3 shows the resulting equipotential lines. If this were a topographical map it would indicate the presence of a narrow ridge along the center spine of the crystal. A significant feature of the equipotential lines on all surfaces containing the most highly conducting b -axis is that they have a very strong tendency to lie parallel to this direction.‡ Therefore, when the current is generally parallel to the b -axis, as in Fig. 2, it is virtually impossible to fabricate a contact which will establish equipotential lines perpendicular to the b -axis. Conversely, it is understandable that a -axis four-probe measurements are and should be unusually insensitive to contact size and placement.

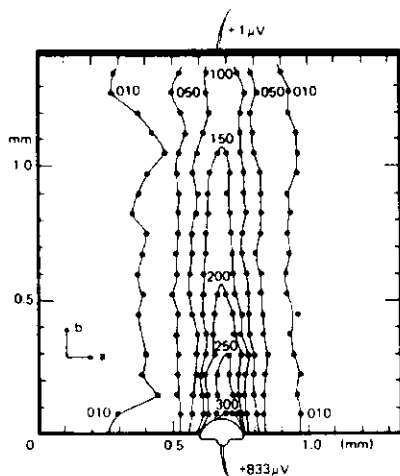


Fig. 3. Potential topography resulting from a line (lower)-plane (upper) contact geometry, with the current generally in the b -direction.

†Cutting was necessary because no crystals having the desired shape (and also natural faces which were exactly perpendicular to the b -axis) were available. If the blade is very sharp, the damage to the crystal is negligible, insofar as its effect on contact resistance is concerned.

‡This same effect was observed by Zosel *et al.* [6] in crystals of much lower conductivity but very large anisotropy.

By comparison of Figs. 2 and 3 it can be seen that the curves of the former could be synthesized by a suitable superposition of curves like those in the latter. This could be done by assuming that there are several small contacts along both surfaces, and by using the number of contacts and their horizontal position as adjustable parameters. This procedure amounts to constructing a simple model of contacts which have microscopic variations in resistivity along their surface. The variations among the curves of Fig. 2 can be accounted for by assuming that each new contact has a different microstructure from that of its predecessor.

The fact that the interfacial resistance fluctuates along the surface of a contact makes it clear why the contact resistances vary widely from sample to sample. During the course of our measurements of the conductivity of many crystals in their three principal crystallographic directions, we made many determinations of contact resistance. Dividing these values by the area of the respective contact (impossible to measure accurately because of their small size and irregular shape) we obtained widely scattered values. Two observations which seem to be of some significance can be made about the results. First, for each crystallographic direction there seems to be a maximum value of contact conductance per unit area of the current-carrying interface. Second, this maximum seems to have the same value (20 mhos/mm²), independent of the crystallographic orientation of the contact plane. In other words, the interfacial contact resistance is approximately isotropic.

During the course of these studies we obtained reproducible values for the diagonal elements of the room temperature conductivity tensor. They are:

$$\sigma_b = 440 \pm 15 \Omega^{-1} \text{cm}^{-1}$$

$$\sigma_{c^*} = 12.6 - 30.0 \Omega^{-1} \text{cm}^{-1}$$

$$\sigma_a = 1.30 \pm 0.05 \Omega^{-1} \text{cm}^{-1}$$

These values were averaged over approximately ten determinations, with the exception of σ_{c^*} (three). The large spread in the values for the latter direction is a consequence of the crystal morphology. The crystals are so thin in the c^* -direction that it is virtually impossible to place two potential contacts on a plane which contains the c^* -direction. If the potential contacts are placed on the a - b surface near the current electrodes, it is very likely that they will detect an erroneous potential, due to effects illustrated in Fig. 2. We believe the lowest value quoted above (12.6) to be the most accurate one. It was obtained from the one crystal on which we were able to measure potential at accurately measured positions along a line parallel to c^* .

Techniques for measuring the principal components of the conductivity tensor from the same sample (e.g. the Montgomery technique[5]) purposely introduce a nonuniform current distribution in the sample. The basic approach is to use a simple well-defined sample shape (generally a rectangular parallelepiped) and to position the contacts (generally assumed to be points) in such a manner that a few simple boundary conditions describe

the current flow in the sample. Then one sets up a suitable array of virtual charges in infinite space which would create these boundary conditions. From this array of image charges one calculates the electrostatic potential at any point on the sample by a series summation.

The contact arrangement shown in Fig. 3 is amenable to the same kind of analytical treatment. The contacts can be approximated by a line parallel to c^* on one b -face, and a plane on the opposite b -face. The boundary conditions are that the current has no horizontal component at the plane contact, and no vertical component at the opposite interface, except at the contact itself. It is also assumed that the current distribution is independent of distance normal to the crystal surface (i.e. along the c^* -axis). For the case that the sample is infinite in the a -direction, the analysis of potential vs distance from the line contact along a normal to the plane contact is relatively simple. It yields the solid curve shown in Fig. 4. The circles are experimental points taken from the data plotted in Fig. 3.

From Fig. 4 it can be seen that a calculation pertaining to a sample of infinite width agrees with data taken from a sample of limited width. One reason is that the square anisotropic crystal is equivalent to an isotropic crystal which is x times as long in the horizontal a -direction, where

$$x = (\sigma_b/\sigma_a)^{1/2} = 18.4.$$

The equivalent isotropic sample, having a dimensional ratio of 18/1, is a much closer approximation to a semi-infinite slab than is a square. This transformation, based on the work of Van der Pauw[8], is an essential feature of the image charge method of analysis. Since the entire surface of the crystal undergoes the same transformation, the equipotential map of Fig. 3 would be stretched sideways in the equivalent isotropic sample. This would have the effect of softening the sharpness of curvature of these curves near the line contact.

The equipotentials calculated for 150, 200 and 250 μ V by using the method of images are shown in Fig. 5. The

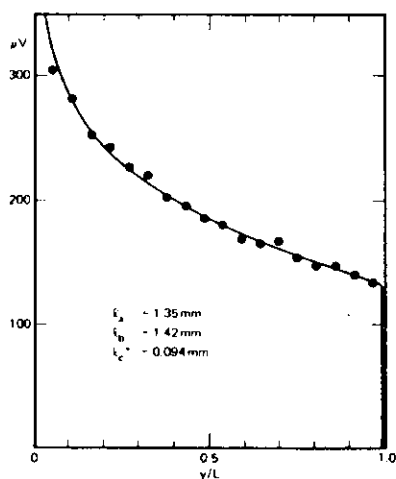


Fig. 4. Comparison of the potential calculated from the image charge model (solid line) with experiment (circles) for points along the b -axis between the contacts of Fig. 3.

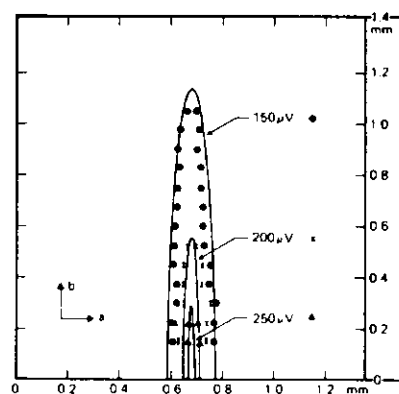


Fig. 5. Comparison of calculated equipotential curves (solid) with experimental points for the central region, in the experiment of Fig. 3.

corresponding experimental points are also shown. Considering the fact that only two parameters have been adjusted to fit the model to the real case (e.g. the two required in Fig. 4), the agreement is remarkably good in this central region of the sample. The anisotropy ratio was taken to be the experimentally determined value of 18.4. However, the agreement between model and experiment is not good for positions relatively far from the central axis. We believe that this effect is due to the presence of the resistive contact layer, which invalidates the assumption of the model that the upper surface of the crystal is an equipotential plane. While this assumption is approximately true near the central axis, it becomes a poorer approximation the farther one goes from the axis.

Another indication that the sample of Figs. 3 and 4 is behaving like a semi-infinite slab is that the entire potential topography lies in the central part of the sample. In other words, the sides of the crystal are at the same potential as the ground contact. The addition of any further amount of sample at the sides would not affect the pattern. For all intents and purposes it might as well be infinite.

The agreement between experimental points and the curves in Figs. 4 and 5 can be taken as a verification of the validity of the assumptions underlying the Montgomery technique. However, it should be pointed out that the equipotential pattern is extremely sensitive to the contacts, especially the small contact. The narrower this contact, the better the result. Reproducibility is a serious problem. It took several careful attempts to obtain a potential pattern as symmetrical with respect to the center line as is that of Fig. 3. From this it can be concluded that extreme care must be exercised in applying contacts for the Montgomery technique. They should approximate point or infinitely narrow line contacts as closely as possible.

The very large potential (130 μ V) measured just off the plane contact and directly opposite the line contact (Fig. 4) is a manifestation of the nonuniform current flow from plane contact to crystal. The large potential results from the large current density flowing through the thin resistive contact layer in that immediate area. It is possible to calculate the current distribution as a function of position

on the plane contact in Fig. 5. Making use of the a -axis, the current distribution can be calculated. From the fact that the current density is inversely proportional to the resistive layer thickness, the contact resistance is 50 mhos/mm², the 20 mhos/mm² gross contact resistance is 2.5 times that of the plane contact.

Because this is a theoretical equipotential surface, it need not have potential sources or sinks. Others based on the same principle are minimized by the presence of the resistive layer.

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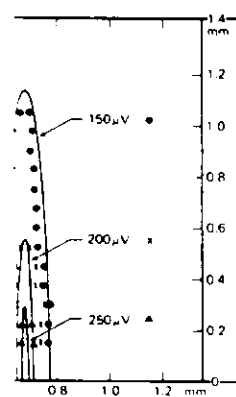
The conclusion is that the measurements are in good agreement with the theoretical model.

(1) The contact resistance is 50 mhos/mm².

(2) The contact resistance is 2.5 times that of the plane contact.



Fig. 6. Potential (left) contact ground.



ed equipotential curves (solid) with central region, in the experiment of Fig. 3.

tal points are also shown. Only two parameters have been taken into the real case (e.g. the two parameters) and the agreement is remarkably good in the experiment. The anisotropy ratio was experimentally determined value of 18.4. The agreement between model and experiment is relatively far from the central region due to the presence of a thin resistive layer which invalidates the assumption that the upper surface of the crystal is an equipotential surface. This assumption is approximately valid along the central axis, it becomes a poorer approximation as one goes from the axis.

In the sample of Figs. 3 and 4 the finite slab is that the entire width of the central part of the sample. The equipotential lines of the crystal are at the same potential. The addition of any other contacts on the sides would not affect the potential distribution as well as

the experimental points and the agreement can be taken as a verification of the model. It is underlying the Montgomery technique could be pointed out that the potential is extremely sensitive to the location of the central contact. The narrower this contact, the higher the potential. Reproducibility is a serious problem. Careful attempts to obtain a uniform potential are necessary. From this it can be concluded that care should be exercised in applying contacts for future experiments. They should approximate the location of line contacts as closely as possible.

(130 μV) measured just off the central axis opposite the line contact (Fig. 5). The nonuniform current flow from the large potential results from the current flowing through the thin resistive layer mediate area. It is possible to calculate the current density as a function of position

on the plane contact for the potential distribution shown in Fig. 5. Making use only of the results near the central axis, the current density in this region can be calculated. From the fact that the measured potential drop across the resistive layer is 130 μV on the central axis, we calculate that the contact conductance per unit area in this region is 50 mhos/ mm^2 . It is interesting that this value is close to the 20 mhos/ mm^2 found experimentally by determining gross contact resistances of a number of samples.

Because this thin resistive layer is present, the surface of a crystal bonded by a metallic contact need not be an equipotential surface, and the current flowing through it need not have uniform current density. This effect is a potential source of error for the Montgomery method (and others based on image charges). These problems can be minimized by making the contacts extremely small.

If the experiment of Figs. 3 and 4 is repeated with the contacts on a -faces, quite different results are obtained. The equipotential lines are parallel to the b -direction, as before. This time, however, they are parallel to the faces bearing the contacts. This time the dimensional transform effectively *squeezes* the sample in the b -direction 18 times with respect to the a -direction. A sample which by physical dimensions is 1.65 times as wide as it is high transforms into one which is not quite 1/10 as wide. One-tenth is a very poor approximation to infinity. The theoretical curve for the line-(infinite plane) case is the same as that shown in Fig. 3. The actual curve (Fig. 6) is linear except for the region very close to the line contact. This is exactly what the calculated curve looks like for a finite sample of this geometry. The slope of the line can be used to calculate the resistivity, as though both contacts were planes covering the end surfaces. This experiment demonstrates the insensitivity of standard conductivity measurements to contact placement in the most resistive direction of anisotropic crystals.

CONCLUSIONS

The conclusions which can be drawn from these measurements at room temperature are:

(1) The contact between silver paint and a TTF-TCNQ crystal behaves like a thin resistive layer. Its surface

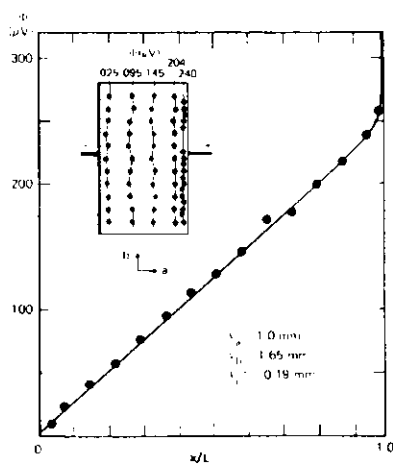


Fig. 6. Potential topography resulting from a line (right)-plane (left) contact geometry, with the current generally in the a -direction.

conductance (≤ 20 mhos/ mm^2) generally varies more or less randomly over the interface. In circumstances of nonuniform current distribution, this resistive layer will result in the crystal surface (under the contact) having a nonuniform potential. Even if the contact layer itself were uniform, the crystal surface would not be equipotential.

(2) The room temperature values of resistivity for our TTF-TCNQ crystals are: $\sigma_b = 440 \pm 15$, $\sigma_c \approx 13$, $\sigma_a = 1.30 \pm 0.05 \Omega^{-1} \text{cm}^{-1}$. These values are completely independent of any contact effects.

(3) Comparing measurements made by the standard four-probe technique on highly anisotropic crystals, those taken with current flow parallel to the conducting b -axis are most subject to error due to contact placement and nonuniformity. Chances of error are smallest with samples of the largest possible aspect ratio; i.e. ones which are as needle-like as possible.

It is difficult to obtain accurate measurements in the c^* -axis direction for a different reason: namely, because TTF-TCNQ crystals grow in platelets normal to this axis. It is important to place the potential contacts on a crystal face containing the c^* -direction. Otherwise one will encounter difficulties of the type illustrated in Fig. 2. The physical difficulty of placing the contacts on the b - c^* face, for example, is alleviated somewhat by the insensitivity of the equipotential lines to displacement along the b -direction. In other words, the potential contacts do not have to be aligned along c^* .

(4) When making measurements by techniques which purposely introduce current distortions into the sample (e.g. Montgomery technique), one must be particularly careful to observe the boundary conditions on which the analysis is based. That means the sample should be shaped accurately, with the optimal dimensional ratios being properly maintained. The contacts should be as small as possible (i.e. approximate point contacts) and meticulously placed on the corners. Otherwise, the contact conductance will upset the boundary conditions.

Finally, a few observations will be made about low temperature measurements. We report no direct low temperature data here because our technique is not applicable in the temperature range of interest (75°K and below). However, two low temperature results reported in the literature, coupled with our room temperature data, allow us to predict that the unintentional current- and field-distortion patterns in b -axis samples (see Fig. 2) would be even worse at low temperature.

First of all, Fig. 2 of Cohen *et al.*[1] shows that the contact resistance at 60°K is larger than that at room temperature by a factor of approximately three. This factor becomes much larger at lower temperatures. In the experiments of our Fig. 2 we found that interfacial resistance fluctuations, and hence distortions of patterns, increased with the gross contact resistance. Secondly, the conductivity anisotropy of TTF-TCNQ is much larger in the region of 60°K than it is at room temperature. For a given b -axis sample with its contacts, distortion of the potential pattern increases with increasing anisotropy.

These comments must stop short of making any prediction about the magnitude of the much-discussed conductivity peak[1-4] or the "anisotropy double maximum,"

which has been attributed to inhomogeneous currents [1]. They are intended merely to point out that the difficulty of obtaining accurate b -axis conductivity values is much greater in the environs of 60°K than it is at room temperature.

Acknowledgements—We wish to thank Dr. George A. Castro for having grown and supplied us with the large pure crystals without which this investigation would have been far more difficult.

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