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# Electric Fields of Defects in Solids

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Explicit consideration is given to the magnitudes of electric fields which exist in nonmetallic solids containing charged defects. Several types of defects are mentioned, and detailed treatment is given to the case of point charges in semiconductors. For this case, probability distributions of the field strengths are found by using the results of the analogous problem in weakly ionized plasmas. The dependence on impurity concentration and the effect of screening by free carriers are shown. The principal conclusion is that most nonmetallic solids are pervaded by high fields—$10^4$ V/cm being a typical average.

## I. INTRODUCTION

It is well known that applied electric fields can affect many of the properties of nonmetallic solids. For example, 10 V/cm is enough to cause avalanche breakdown in semiconductors at very low temperatures[1]; $10^3$ V/cm substantially alters the recombination statistics for photocurrent in cadmium sulfide[2] and causes measurable hot electron effects in semiconductors[3]; $10^5$ V/cm shifts the fundamental optical absorption edge.[4] In spite of these, and other, effects of externally applied fields, little attention has been given to the corresponding effects which may be caused by naturally occurring fields that are known to arise at charged defects in solids. Such charges may occur at points (impurities or lattice defects), lines (dislocations), or planes (surfaces or junctions). It will be shown elsewhere that defect fields do produce significant effects, and these can account for some previously unexplained observations. To evaluate such effects, however, explicit values of the field strengths are needed. It is the purpose of this paper to present these field strengths with emphasis on the case of point charges because it is generally the most important one (of the fixed defects) and has not been discussed previously. The time-varying fields due to lattice vibrations in ionic crystals are essentially different and will be treated in a later paper. In this discussion it is understood that the average field is zero when sign is considered, but all further references to fields will be to the *magnitudes*, whose average is not zero.

## II. SURFACES AND DISLOCATIONS

These are mentioned here chiefly for the sake of completeness since the fields can be easily obtained from published work on the potential distributions near charged dislocations and surfaces. These are almost always treated as noninteracting space-charge regions and the derived potential distributions are straightforward. Charged dislocations have been treated approximately for semiconductors[5] and insulators,[6] while the space-charge region near a semiconductor surface has been considered in more detail.[7] Effects due to surfaces will clearly be more important for thin samples than for thick ones, and in thin films may well dominate some properties. In any case, peak field strengths in excess of $10^5$ V/cm are commonly found and space-charge layer thicknesses are often between 100 Å and 1 $\mu$.

## III. POINT CHARGES

The distribution of electric field strengths in a solid containing charged point defects has apparently not been considered explicitly and will be discussed here in some detail. It is assumed that there are $N$ singly charged defects per $cm^3$, randomly placed in a medium of static dielectric constant $\epsilon$. All are considered to have the same sign, their charge being compensated by free carriers in semiconductors or additional defects in insulators. The usual approximations[8] involved in the use of the static dielectric constant to represent the crystal lattice are also implied here. It will turn out that the small regions close to the charges where this in invalid do not contribute greatly to most of the effects.

For many purposes, the most useful way to express the desired result is as the probability $W(F)dF$ of finding a field of magnitude $F$. When normalized to unity, this is the fraction of the volume of a crystal occupied by fields in the range $dF$. Stated in this form, the present problem is identical to that found in the quasi-static approximation for the calculation of electric field distributions in weakly ionized plasmas, and of gravitational field distributions in stellar dynamics. The results obtained in these other areas will now be used in the form appropriate to the present problem. As a first approximation, consider the probability of finding a field $F$ at any general point in a crystal neglecting all contributions except that due to the Coulomb field of the nearest charge. This "nearest ion distribution" can be readily found from the position

[1] N. Sclar and E. Burstein, J. Phys. Chem. Solids **2**, 1 (1957).
[2] S. Kitamura, T. Kubo, and T. Yamashita, J. Phys. Soc. Japan **16**, 351 (1961).
[3] J. B. Gunn, J. Electron. **2**, 87 (1956).
[4] Richard Williams, Phys. Rev. **126**, 442 (1962).
[5] W. T. Read, Phil. Mag. **45**, 775 (1954).
[6] J. D. Eshelby, C. W. A. Newey, P. L. Pratt, and A. B. Lidiard, Phil. Mag. **3**, 75 (1958).
[7] For a recent review, see T. B. Watkins, in *Progress in Semiconductors*, edited by A. F. Gibson *et al.* (John Wiley & Sons, Inc., New York, 1960), Vol. 5, p. 1.
[8] W. Kohn, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957), Vol. 5, p. 257.

distribution function of random points.[9] It is most simply expressed in terms of a "normal distance" $r_0$ defined so that $(4\pi/3)r_0^3 = N^{-1}$. Thus, $r_0$ is the radius of a sphere whose volume equals the mean volume per defect; also, $r_0 = 0.62N^{-1/3}$, where $N^{-1/3}$ is just the unit separation of $N$ defects arranged in a cubic array. The "normal field" is then defined by

$$F_0 \equiv e/\epsilon r_0^2 = 2.6(e/\epsilon)N^{2/3}, \qquad (1)$$

where $e$ is the magnitude of the electronic charge. In terms of this $F_0$, the nearest ion distribution is[9]

$$W(F)dF = \frac{3}{2F}\left(\frac{F_0}{F}\right)^{3/2} \exp\left[-\left(\frac{F_0}{F}\right)^{3/2}\right]dF. \qquad (2)$$

This function is shown as the dashed line in Fig. 1 where $W$ is plotted as a function of the reduced field $\beta = F/F_0$.

To obtain a distribution function which considers contributions from all the charges added vectorially at any general point, Holtsmark[10] used the method of Markoff and obtained the solution shown graphically with his name in Fig. 1. This has been used very successfully in astronomy and for plasmas of moderate density. For the present purposes the only modification of the Holtsmark distribution needed is due to the screening effect of free electrons or holes in semiconductors. The reamining two curves of Fig. 1 illustrate the effect of screening and its dependence on the ratio of $r_0$ to $\lambda$ the Debye length.[11] It should be noted that all the curves of Fig. 1 merge at high fields and fall off as $F^{-5/2}$. This fairly rapid decrease is due to the fact that the higher fields exist only in relatively small volumes close to the charges.

The magnitudes of the fields in any case are determined simply by $F_0$ which acts like a scale factor for the distribution functions. For a semiconductor of fair purity with $N \sim 2\times10^{17}$ cm$^{-3}$, and taking $\epsilon = 12$, Eq. (1) gives $F_0 \sim 10^4$ V/cm and $r_0/\lambda = 1.1$. Although distribution curves for such values of $r_0/\lambda$ are not available, the trend of Fig. 1 indicates that the nearest ion distribution will be a good approximation for this case and (because of the weak dependence[11] of $r_0/\lambda$ on $N$) for a considerable range of $N$. It is easily shown, furthermore, that the average field for the nearest ion function is $\langle F\rangle = 2.7\ F_0$ and it can be seen by inspection of Fig. 1 that this must be roughly the same for a moderately screened Holtsmark distribution. In fact, the average field will not be highly sensitive to the impurity concentration because screening effects partially offset changes in $F_0$.

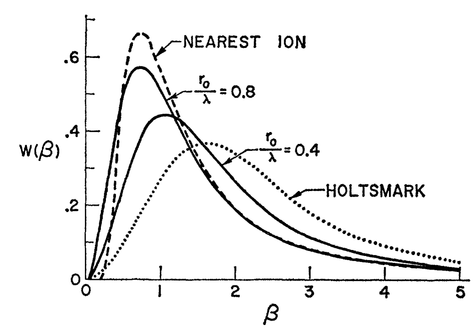


FIG. 1. Probability distributions of electric field strength for several cases. $\beta = F/F_0$.

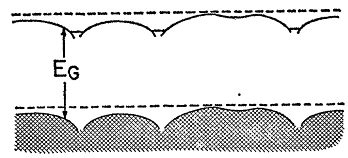


FIG. 2. Preferred energy band diagram of a semiconductor with charged donors. Emphasis is on the fluctuating level of the band edges (shown in exaggerated amounts). The dip appearing between two donors illustrates the influence of a nearby donor not in line with the other three donors.

## IV. DISCUSSION

It is apparent, therefore, that most materials are pervaded by fields of considerable strength. That the effects of these fields can be significant will be shown elsewhere. In the following paper, for example, these fields are invoked to explain the "Urbach rule" tails on fundamental optical absorption edges. The one further point to be noted here is that the existence of these fields is obscured by the customary diagrams of flat energy bands with adjacent localized levels of the defects. Figure 2 shows a better illustration of the situation—one that has been long known, but usually not used.

Finally, mention should be made of insulators which normally have fixed defects with charges of both sign. Field distributions in such regions have not been derived except for the case in which positive and negative defects associate in pairs. This would produce dipolar fields, also treated by Holtsmark.[12] The distribution function in this case is similar to the ion field distribution but the normal field is given by $F_0 = 4.54\ \mu N$, where $\mu$ is the individual dipole moment. No further discussion of these fields in insulators will be given here, however, because there is reason to believe that the polarization waves caused by lattice vibrations in ionic crystals are more important. These will be treated in a later paper.

[9] For example, see H. Margenau and M. Lewis, Rev. Mod. Phys. **31**, 569 (1959).

[10] J. Holtsmark, Ann. Physik **58**, 577 (1919). For a discussion of this and other stochastic problems, see S. Chandrasekar, Rev. Mod. Phys. **15**, 1 (1943).

[11] M. Baranger, in *Atomic and Molecular Processes*, edited by D. R. Bates (Academic Press Inc., New York, 1962). For this case $\lambda = (\epsilon kT/4\pi Ne^2)^{1/2}$ so that $r_0/\lambda \propto N^{1/6}$.

[12] For a discussion of this, see R. G. Breene, Rev. Mod. Phys. **29**, 94 (1957).