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A Possible Explanation of the Observed Electron Drift Velocity Saturation in Solid Ar, Kr, and Xe

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The recently published drift velocity measurements of excess electrons in solid Ar, Kr, and Xe show a complete saturation of the drift velocity with applied field between 10^4 and 10^5 V cm^{-1}. In this paper it is suggested that the interaction of the conduction electrons with the periodic structure is the basic velocity-limiting mechanism in these solids. The model is supported by a simple calculation in which an energy-dependent effective mass is included in the Shockley hot electron theory. The computed field dependence of the drift velocity, involving one adjustable parameter, is in good agreement with the observed curves for solid Ar, Kr, and Xe over the complete range of applied fields.

1. INTRODUCTION

In a recent paper[1] we reported the results of drift velocity measurements of excess electrons in solid and liquid Ar, Kr, and Xe over a wide range of applied fields. An interesting feature was the occurrence of pronounced hot electron effects which in the low- and intermediate-field range could be accurately fitted to the well-known Shockley theory.[2]

However, with increasing applied field, all the results showed marked deviations from the Shockley theory which eventually led to a complete saturation of the drift velocity v with the applied field E. This behavior is illustrated by the experimental points in Figs. 1 and 2 for solid Ar and solid and liquid Kr, respectively. The graphs also include the saturation velocities recently obtained by Pruett and Broida[3] which are in good agreement with our measurements and extend the field range to higher values.

Table I lists the low field mobilities μ_0 near the triple-point temperature and also gives the saturation velocity v_s in terms of the velocity of sound u in the medium. There is a systematic decrease of v_s/u from Ar to Xe and also the deviation from the $E^{1/2}$ dependence predicted by the Shockley theory (line S in Figs. 1 and 2) occurs at progressively lower values of E.

A possible explanation for the observed velocity saturation is provided by a more general hot electron theory recently developed by Cohen and Lekner.[4] Their treatment is based on a solution of the Boltzmann equation and does not involve the assumption of a heated Maxwellian distribution. It also takes account of the structural properties of the medium in which the electrons propagate; the structure factor $S(k)$, which is proportional to the effective scattering cross section, enters the expression for the mean free path involved in the momentum transfer on scattering. On the basis of this theory, Lekner[5] has carried out detailed calculations for the case of liquid Ar. The predicted v-E curve is in good agreement with the experimental points, up to fields of about 20 kV cm^{-1}, beyond which it shows a marked decrease in v rather than the observed saturation. Pruett and Broida,[3] on the other hand, put forward the suggestion that the velocity saturation was due to the effect of inelastic scattering by molecular impurities such as N_2, O_2, etc. Their experimental evidence, in agreement with our own results, shows that the deliberate addition of such impurities leads to an increase in the saturation level, caused by a cooling of the electron distribution. It is, however, difficult to understand how such a mechanism could be the fundamental reason for the complete velocity saturation over a wide field range, observed consistently in all rare gas crystals.

We should like to suggest that the interaction of the conduction electrons with the periodic structure is the basic velocity-limiting mechanism in the rare gas crystals. The main purpose of the following highly simplified calculation is to demonstrate that, if this interaction is included in terms of an effective mass approximation, a consistent explanation of the observed effects can be obtained.

TABLE I. Summary of relevant data for the rare gas solids and liquids. μ_0 is the low-field electron mobility from Ref. (1) at the stated temperatures close to the triple points. vs/u is the saturation velocity expressed in terms of the sound velocity u. The listed values of W gave the best fit to the experimental curves.

	T (°K)	μ_0 (cm^2 sec^{-1} V^{-1})	u (10^5 cm sec^{-1})	$\left(\frac{v_s}{u}\right)$	W (eV)
Solids					
Ar	82	1000	1.38[a]	10	0.36
Kr	113	3600	1.28[b]	6.8	0.22
Xe	157	~4000	~1.1[c]	5.0	~0.2
Liquids					
Ar	85	475	0.86[d]	9.4	0.30
Kr	117	1800	0.7[d]	5.4	0.14
Xe	163	1900	0.65[d]	4.4	0.14

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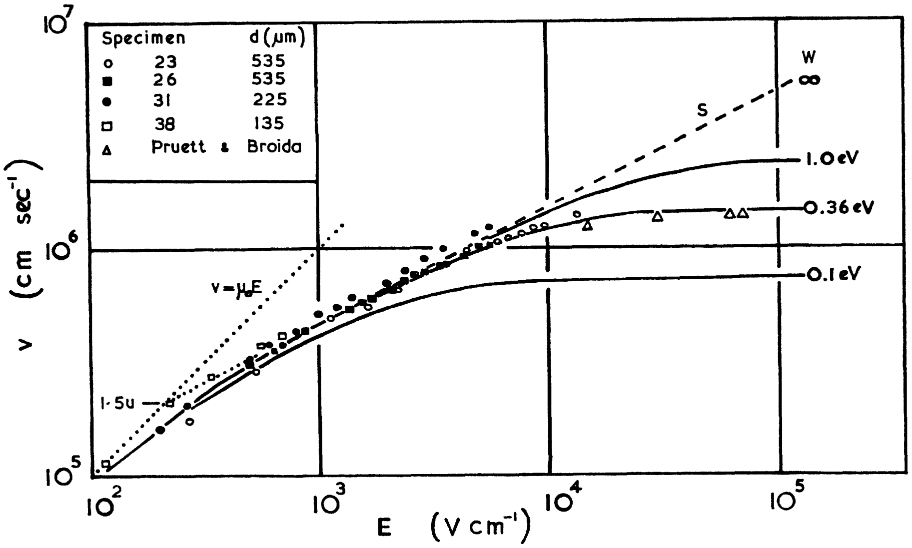

FIG. 1. The field dependence of the electron drift velocity in solid Ar at 82°K. The experimental results for a number of specimens are compared with the calculated curves (solid lines) for different values of the parameter W. Curve S ($W=\infty$) shows the $E^{1/2}$ dependence predicted by the Shockley theory.

2. THEORY INCLUDING AN ENERGY-DEPENDENT EFFECTIVE MASS

The Shockley theory forms the basis of the calculation. Although there exists considerable doubt concerning the general validity of the effective temperature concept, the satisfactory agreement of the theory, particularly with the Ar results, suggests that its application in the case of rare gas crystals should be a reasonable approximation.

The drift velocity, determined by acoustic scattering, is given at low applied fields by

$$v_0=\mu_0E=[4el_0/3(2\pi m_0{}^*kT)^{1/2}]E, \tag{1}$$

where l_0 and $m_0{}^*$ denote the mean free path and the effective mass near the bottom of the conduction band and T is the lattice temperature. Optical phonon scattering does not occur in the fcc lattice of the rare gas crystals. When the field is increased, the electron distribution heats up and is now described by an effective temperature T_e. The effective mass will increase with electron energy and the mean free path is likely to decrease. The drift velocity then becomes

$$v=\mu_0E\gamma^{-1/2}\left(\frac{m_0{}^*}{m^*}\right)^{1/2}\left(\frac{l}{l_0}\right), \tag{2}$$

where

$$\gamma=T_e/T.$$

The average energy of the electrons is given by

$$\epsilon=\tfrac{3}{2}kT_e=\tfrac{3}{2}kT\gamma. \tag{3}$$

γ is calculated by equating the rate of energy gain by the conduction electrons to the rate of energy loss by acoustic scattering. This leads to

$$\gamma^2-\gamma=\frac{3\pi}{32}\frac{m_0{}^*}{m^*}\left(\frac{l}{l_0}\right)^2\left(\frac{\mu_0E}{u}\right)^2. \tag{4}$$

The problem of how to express the energy dependence of

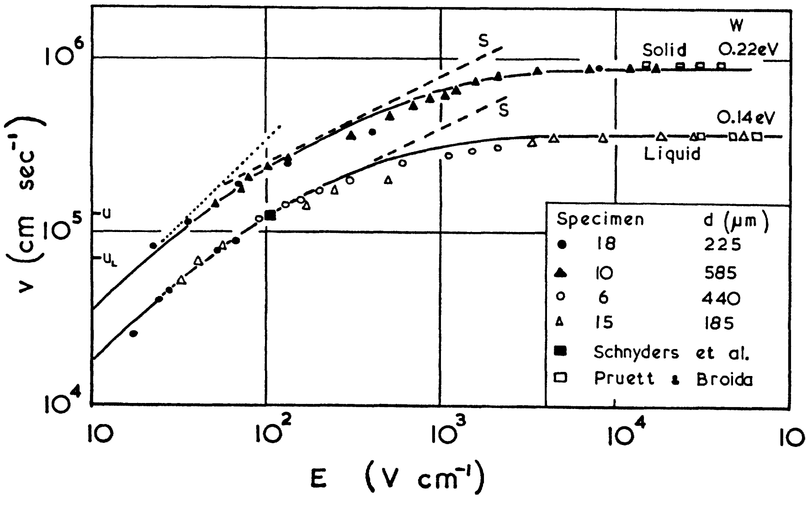

FIG. 2. The field dependence of the electron drift velocity in solid Kr (113°K) and liquid Kr (117°K). The solid lines have been calculated using the indicated values of W. Curve S was calculated from Shockley theory.

m_0^*/m^* and of l/l_0 now arises. Band structure calculations have been carried out for Ar,[6,7] Kr,[8] and Xe.[9] The bottom of the conduction band lies at the Γ point in all cases and there exists a marked similarity in the shape of the conduction bands calculated for the three rare gas solids. Their widths decrease progressively from about 3 eV in Ar to 2 eV in Xe. In the present calculation the following, admittedly crude, approximation has been used to express the energy dependence of m_0^*/m^* in the lower half of the conduction band in simple analytical form. Starting from the well-known tight-binding approximation,[10] it can easily be shown that for cubic structures the ratio m_0^*/m^* (assumed isotropic) is given by an expression of the form

$$m_0^*/m^* = 1 - \epsilon/W = 1 - \tfrac{3}{2}kT\gamma/W. \qquad (5)$$

W is regarded here as an adjustable energy parameter which will depend on the more detailed shape of the conduction band, the anisotropy of m^*, and possibly also on deviations from the Maxwellian distribution as the electrons become hot. Its value should be such that near $\epsilon = W$, $\partial\epsilon/\partial k$ tends towards a constant value, which means that m^* will rise rapidly near that energy. The published bandshapes suggest that this condition is approached at energies below the center of the bands and one would expect W values less than about 0.7 eV.

As far as the energy dependence of the mean free path in rare-gas media is concerned, we would like to suggest that $l/l_0 \simeq 1$, at least within the context of the present simple treatment. This assumption is based on the detailed calculations of the electron scattering cross section in liquid Ar carried out by Lekner.[5] The results show that the cross section, and hence the mean free path, is practically independent of electron energy, even when ϵ approaches a few eV. The remarkable similarity between the transport properties of solid and liquid rare gases (see Table I) suggests that this is likely to apply also to the crystalline case considered here. Also, any moderate deviation from the approximation $l/l_0 \simeq 1$ should only affect the calculated v-E curves in the intermediate field range, because within the scope of the present treatment the saturation velocity is found to be independent of l/l_0 (Eq. 6).

Equations (4) and (5) now lead to values of γ and of m_0^*/m^* at any given E; by substitution into Eq. (2) the corresponding drift velocity is obtained. Figure 1 shows the computed v-E curves for several values of W. $W = 0.36$ eV gives an excellent fit to the observed points in solid Ar over the complete experimental range of E. Figure 2 shows equally good agreement in the case of the solid Kr data. The W values used, which are included in Table I, decrease from Ar to Xe and thus show the same trend as the band widths.

In the saturation region, $\gamma^2 \gg \gamma$, so that the linear term in Eq. (4) can be neglected, which allows us to derive the following simple expression:

$$v_s/u = (32/3\pi)^{1/2}(2W/3kT)^{1/2}. \qquad (6)$$

v_s/u is thus independent of the mobility and of l/l_0 and should increase with decreasing lattice temperature. Experiments are in progress to investigate this temperature dependence.

In view of the success of the present model for the rare gas crystals it seems tempting to test its applicability to the liquids. However, it is by no means obvious that some of the concepts used above can be applied to the liquid state and this would need more justification. Nevertheless, the exceptionally high mobilities of these liquids (see Table I), the striking similarity of the experimental curves and of the v_s/u ratios to those for the corresponding solids suggests that there may be little fundamental difference between the transport properties in the two states. Figure 2 shows the fit in the case of liquid Kr, but as indicated in Table I, the required W values are appreciably lower than for the corresponding solids.

3. SUMMARY

It has been shown that if the changes in effective electron mass with energy in the lower half of the nonparabolic bands are included, the Shockley hot-electron theory leads to good agreement with the experimental v-E curves for solid Ar, Kr, and Xe over the complete field range. The important point that emerges from the simple calculation is that as the average electron energy approaches a limiting value W, the expected rise in v with E is almost exactly balanced by the effect of the increase in m^*. This leads to the complete velocity saturation observed in all experiments without the need for additional assumptions. The values of W required for the fit are somewhat low as compared to the bandwidths, but in view of the highly simplified expression for the energy dependence of m^*, it is doubtful whether a direct physical meaning can be attached to the magnitude of this parameter at present. We believe, however, that it would be worth while to carry out a more detailed calculation of the energy dependence of m^* on the basis of the band structure data.

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