tional to

 $\tau^2 = \tau_c \tau_H = \frac{3 \mu_H \mu_c}{e^2}$ 

relaxation time  $\tau_c$  is related to the drift mobility by  $^{10,11}$ 

$$
\tau_c = \int_0^\infty \tau \epsilon^{3/2} f^0 d\epsilon / \int_0^\infty \epsilon^{3/2} f^0 d\epsilon
$$

$$
= \mu_d / \frac{1}{3} e \left( \frac{1}{m_1^*} + \frac{1}{m_2^*} + \frac{1}{m_3^*} \right). \tag{D1}
$$

Similarly, the Hall relaxation time  $\tau_H$  is related to the Hall mobility  $\mu_H (=R\sigma_0)$  by

$$
\tau_{H} = \int_{0}^{\infty} \tau^{2} \epsilon^{3/2} f^{0} d\epsilon / \int_{0}^{\infty} \tau \epsilon^{3/2} f^{0} d\epsilon
$$

$$
= \frac{\mu_{H}}{e} \left( \frac{1}{m_{1}^{*}} + \frac{1}{m_{2}^{*}} + \frac{1}{m_{3}^{*}} \right) / \left( \frac{1}{m_{1}^{*} m_{2}^{*}} + \frac{1}{m_{2}^{*} m_{3}^{*}} + \frac{1}{m_{1}^{*} m_{2}^{*}} \right). (D2)
$$

<sup>10</sup> C. Herring, Bell System Tech. J. 34, 237 (1955); C. Herrin and E. Vogt, Phys. Rev. 101, 944 (1956).<br><sup>11</sup> J. C. Hensel, Phys. Rev. 129, 1041 (1963).

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# Hall Mobility in  $SrTiO<sub>3</sub>$ <sup>†</sup>

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Electron mobilities in reduced and doped  $SrTiO<sub>3</sub>$  have been deduced from measurements of the conductivity and Hall coefficient between 1 and  $1000\textdegree K$ . Above room temperature, scattering by the highest two longitudinal optical modes determines the mobility. Expressions based on intermediate electron-phonon coupling yield good agreement with experimental results. Below 10'K experiments indicate that ionized impurity scattering is the dominant collision process. Using a screened Coulomb potential, one obtains mobility values of the right order of magnitude.

## INTRODUCTION

HE quantitative understanding of electron scattering' in polar semiconductors has progressed somewhat less than that of scattering in covalent semiconductors.<sup>2</sup> This lag is caused by a number of inherent difficulties. At high temperatures, the mobility of electrons in polar semiconductors is often limited by optical mode scattering, which is governed by an electron-

phonon coupling constant  $\alpha^{3,4}$  The parameters that appear in  $\alpha$  are the effective mass of the electron  $m^*$ , the energy of the phonon  $h\omega_{\rm ph}$ , and the high- and low-frequency dielectric constants of the medium,  $\epsilon_{\rm op}$  and  $\epsilon_{\rm stat}$ . So far, very little has been done theoretically to take into account the energy and wave-vector dependence of these quantities. Moreover, the electrons in a polar material have an effective mass different from that calculated on the basis of a rigid lattice. In a polar crystal an electron will cause a local polarization, which will "dress" the electron. Hence the electron- when moving—will take this "polarization-dressing" along. The

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If we now re-examine our formalism, we note that in the nondegenerate limit,  $H_{2i}$  of Eq. (2.21) is propor-

 $\int_{0}^{\infty} \epsilon_i^{3/2} f_i^0 d\epsilon_i.$ 

which can also be obtained from (D1) and (D2) by

 $e^{\frac{2}{\pi}} = \int r^2 \epsilon_i^{3/2} f_i^0 d\epsilon_i / \int \epsilon_i^{3/2} f_i^0 d\epsilon_i$  (D3)

 $\left(\frac{1}{m_1^*m_2^*} + \frac{1}{m_2^*m_3^*} + \frac{1}{m_1^*m_2^*}\right)$ . (D4)

Thus, our  $\tau$  should be defined as

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t Research supported in part by the National Aeronautic and Space Administration.

<sup>&</sup>lt;sup>1</sup>It is noteworthy that the *Proceedings of the International Conference on the Physics of Semiconductors, Kyoto, 1966 [J. Phys. Soc. Japan Suppl. 21 (1966)] do not contain a single paper (experimental or theoretical) de* limited Hall mobilities in semiconductors. ' F.J. Blatt, Solid State Phys. 4, 199 (1957).

<sup>&#</sup>x27; H. Frohlich and N. F. Mott, Proc. Roy. Soc. (London) A171, 496 (1939). ' F. E. Low and D. Pines, Phys. Rev. 98, 414 (1955).

electron becomes a "polaron" and the effective mass of this quasiparticle is larger. '

There are also difhculties of an experimental nature. Plotting the Hall mobility of several polar semiconductors as a function of temperature over a limited temperature range, many experimenters find it difhcult to decide between an exponential behavior and a power law.<sup>6</sup> If the energy of the phonon involved is of the order of 30-70 meV, a plot of log  $\mu$  versus  $1/T$  produces as good (or bad) a straight line as  $\log \mu$  versus  $\log T$  (over  $a$  range of  $T$  around room temperature). In the latter case the power of T is usually between  $-2.5$  and  $-3.2$ . Such a temperature dependence has been observed in covalent, many-valley semiconductors and is attributed to inter-valley scattering involving acoustical modes.<sup>7</sup>

The low-temperature mobility usually is limited by defect scattering, the defects being ionized or neutral impurities, dislocations, grain boundaries, or possibly magnetic ions. To determine the specific nature of the scattering mechanism, one studies the temperature dependence and magnitude of the mobility and compares these with theoretical predictions.<sup>2</sup> The main physical parameters governing the scattering are the electron effective mass and the dielectric constant; however, these quantities are significantly modified as a result of the screening by the electrons themselves and by the host lattice. Comparison of theory with experiment often is hampered by the same kind of difficulties as one encounters at high temperatures. Uncertainties exist with respect to the choices of dielectric constant ( $\epsilon_{op}$  or  $\epsilon_{stat}$  or some value in between), effective mass (bare mass or polaron mass), screening length, cutoff distance, Fermi velocity (in case of anisotropic energy bands), etc.

The subject of this paper—electron mobility in reduced and doped  $SrTiO<sub>3</sub>$ —illustrates the above problems very well. Some years ago, the present authors published data on transport properties in  $SrTiO<sub>3</sub>$  between 4.2 and 300°K.<sup>8</sup> At that time we reached the conclusion that "in the temperature range 100—300'K the mobility is proportional to  $T^{-x}$ , where x is between 2.7 and 3.2." It was suggested that this power of  $T$  is compatible with acoustical lattice scattering taking into account an apparent temperature dependence of the effective mass. The reader was warned, however, that "this reasoning should be regarded with reservations."

More recently a similar temperature dependence of electron mobility was reported by Wemple<sup>9</sup> for  $KTaO<sub>3</sub>$ electron mobility was reported by Wemple<sup>9</sup> for KTaO<sub>3</sub><br>( $\mu \sim T^{-2.7}$ ). In a subsequent letter,<sup>10</sup> Wemple *et al.*, use hydrostatic-pressure experiments as evidence that the electron scattering in  $LMO<sub>3</sub>$ -type semiconductors is caused by the long-wavelength, transverse-optical (TO), ferroelectric lattice mode.<sup> $11$ </sup>) This conclusion is difficult to accept for the following reasons:

1. It has been shown that the electron in  $SrTiO<sub>3</sub>$ couples strongly to the highest two LO modes. Coupling couples strongly to the highest two LO modes. C<br>to a transverse mode usually is much weaker.12

2. I—<sup>V</sup> curves obtained in tunneling experiments showed a strong peak at the energy of the highest longitudinal optic (LO) mode and no TO modes.<sup>13</sup>

3. A recent study of electronic transport in BaTiO<sub>3</sub> around the Curie temperature indicates that the mobility becomes anisotropic but does not show any discontinuity at  $T_c$  as expected when  $\epsilon_{stat}$  would play a major role.<sup>14</sup>

A short time ago Tufte and Chapman" announced measurements on  $SrTiO<sub>3</sub>$  up to  $550^{\circ}K$ , from which they concluded that scattering at high temperatures was dominated by polar optical-lattice modes.

The present paper discusses the electron mobility in  $Nb-$ , La-doped, and reduced  $SrTiO<sub>3</sub>$  as deduced from experiments of resistivity and Hall effect between 1 and 1000'K.

Results indicate scattering by the two highest longitudinal-optical (LO) modes at high temperature and ionized impurity scattering at low temperatures.

## **EXPERIMENTAL**

The Hall coefficient and the resistivity of more than 30 samples have been measured. Some of these specimens were Nb or La doped by addition of  $Nb_2O_5$  or  $La<sub>2</sub>O<sub>3</sub>$  during the growth process. Six samples of this group have been investigated up to 900 or 1000'C in air. The majority of the samples were reduced under a variety of conditions with respect to reducing agent (hydrogen, titanium powder), gas pressure and temperature. Table I gives preparative details and other characteristics of all the samples studied.

The Hall coefficient and the resistivity were determined using a conventional potentiometric method. For the high-temperature measurements, platinum leads were fused to the samples using a Ti-Cu "solder."

# RESULTS AND DISCUSSION

Typical data of Hall coefficient and resistivity as a function of temperature from 4.2 to 1000'K are shown in Fig. 1. The Hall coefficient is approximately independent of temperature. In all samples the charge carriers become degenerate on cooling within this temperature

<sup>&</sup>lt;sup>15</sup> G. R. Allcock, Advan. Phys. 5, 412 (1956).<br>
<sup>6</sup> See, e.g., R. L. Petritz and W. W. Scanlon, Phys. Rev. 97, 1620 (1955).

<sup>&</sup>lt;sup>7</sup> C. Herring, Bell System Tech. J. 34, 237 (1955).<br><sup>8</sup> H. P. R. Frederikse, W. R. Thurber, and W. R. Hosler, Phys Rev. 134, A442 (1964).<br>
<sup>9</sup> S. H. Wemple, Phys. Rev. 137, A1575 (1965).

<sup>&</sup>lt;sup>9</sup> S. H. Wemple, Phys. Rev. 137, A1575 (1965).<br><sup>10</sup> S. H. Wemple, A. Jayaraman, and M. Di Domenico, Jr., Phys. Rev. Letters 17, 142 (1966).

<sup>&</sup>lt;sup>11</sup> R. A. Cowley, Phys. Rev. 134, A981 (1964).<br><sup>12</sup> F. Stern, Solid State Phys. 15, 299 (1963).<br><sup>13</sup> S. Shapiro, Phys. Rev. 140, A169 (1965).

<sup>&#</sup>x27;4 C. N. Berglund and W. S.Beer, Phys. Rev. 157 358 (1967). Receipt of a copy of this paper prior to publication is gratefully acknowledged.

<sup>&</sup>lt;sup>15</sup> O. N. Tufte and P. W. Chapman, Phys. Rev. 155, 796 (1967).

Sample	Reduction temp. $(^{\circ}C)$	Time (h)	Dopant wt. $\%$ oxide to powder	Carrier conc. $4.2^{\circ}$ K $(cm^{-3})$	Mobility at $4.2^{\circ}$ K (cm <sup>2</sup> /V sec)	Activ. energy of mobility (eV)	
HR41 HR39 HR11 HR9 <b>HR56</b> <b>HR48</b> <b>HR35</b> HR49(111) HR49(110) HR55 <b>HR22</b> HR6a <b>HR51</b> <b>HR33</b> <b>HR58</b> <b>HR63</b> <b>HR61</b> <b>HR59</b> N <sub>b</sub> 5, 16 Nb 7 N <sub>b</sub> 8 Nb <sub>9</sub> Nb 10 Nb 11 Nb 12 Nb 15 La 1, 2	725 700 704 770 850 875 725 860 860 950 900 950 1000 1150 1200 1250 1300 1370	22 9 23 26 22 21 20 24 24 28 42 60 23 $\frac{46}{5}$ $\frac{3}{3}$ $\frac{3}{2.5}$	0.05 0.05 0.07 0.15 0.50 1.0 0.10 0.01 0.1	3.5 $\times$ 10 <sup>17</sup> $7.3 \times 10^{17}$ $7.1 \times 10^{17}$ $1.1 \times 10^{18}$ $2.0 \times 10^{18}$ $2.3 \times 10^{18}$ $1.7 \times 10^{18}$ $5.2 \times 10^{18}$ 4.5 $\times$ 10 <sup>18</sup> $6.0 \times 10^{18}$ $1.0 \times 10^{19}$ $2.2 \times 10^{19}$ $9.4 \times 10^{18}$ $6.3 \times 10^{19}$ $7.4 \times 10^{19}$ $1.25 \times 10^{20}$ $1.1 \times 10^{20}$ 5.3 $\times$ 10 <sup>20</sup> $7.4 \times 10^{18}$ 5.7 $\times$ 10 <sup>18</sup> $1.3 \times 10^{19}$ $1.8 \times 10^{19}$ $1.7 \times 10^{20}$ $3.8 \times 10^{20}$ $1.6 \times 10^{19}$ $1.6 \times 10^{19}$	13 000 7520 6960 4900 6000 7290 10 400 4300 2050 1470 2300 1040 1609 368 316 185 228 67 7970 8880 5330 4510 613 206 3250 4115	0.108 0.062 0.101 0.057 0.121 0.057	
La <sub>3</sub>			0.025	$3.1 \times 10^{18}$		0.103 0.062	

TABLE I. Characteristics of reduced and doped  $SrTiO<sub>3</sub>$  samples.

range. Consequently, the Hall coefficient contains a scattering factor unequal to 1.0 at high temperatures, while this factor is 1.0 in the degenerate range (e.g., 4.2'K). Hall coefficients at liquid-helium temperatures have been used to calculate the carrier concentration listed in column <sup>5</sup> of Table I.

### A. High-Temperature Range (200-1000'K)

The mobility  $\mu_H$  presented in Fig. 2 is plotted semilogarithmically. Over the temperature range shown here and down to  $100^{\circ}$ K,  $\mu$ <sup>H</sup> does not depend significantly on the impurity content, hence the scattering mechanism



FIG. 1. Electronic transport parameters of reduced (HR-11) and doped (Nb 5 and La 1) SrTiO<sub>3</sub>. (Resistivity: solid lines Hall coefficient: dashed lines.)

must be intrinsic. The data shown in Fig. 2 fall reasonably well on two straight lines. The slopes of these lines correspond to energies of the order of 0.10—0.12 eV and 0.057—0.<sup>62</sup> eV (listed in Table I). These values are very close to the energies of the highest and second-highest longitudinal-optical modes, 0.099 eV and 0.058 eV, longitudinal-optical modes, 0.099 eV and 0.058 eV<br>respectively.<sup>16</sup> Hence, it is worthwhile to check the absolute value of the mobility with theoretical predictions. The optical-mode scattering depends on the electron-phonon coupling constant  $\alpha$ . For the intermediate coupling range  $(1<\alpha<6)$ , Low and Pines<sup>4</sup> derived the following expression:

range (1<
$$
\alpha
$$
<0), Low and Pines<sup>4</sup> derived the  
g expression:  

$$
\mu_{i.e.} = \frac{1}{2\alpha\omega_l} \times \left(\frac{m^*}{m_P}\right)^2 f(\alpha) (e^{\hbar\omega_l/kT} - 1), \qquad (1)
$$

where:

$$
m_P = \text{polaron mass} = m^*(1 + \alpha/6),\tag{2}
$$

and  $m^*$  = (bare) effective mass,  $\omega_l$  = frequency of the long. opt. mode involved, and  $f(\alpha) =$ a function which rises slowly from 1.0 to 1.4 when  $\alpha$  increases from 1 to 6. Equation (1) has to be used twice, for the highest LO mode  $(h\omega=0.099 \text{ eV})$  and for the next lower one ( $\hbar\omega$  = 0.058). The resulting mobilities  $\mu_1$  and  $\mu_2$  are then added reciprocally:

$$
1/\mu = (1/\mu_1) + (1/\mu_2). \tag{3}
$$

For  $m^*$  in Eq. (1), we have chosen the "mobility-mass"

 $\overline{W}$ . S. Spitzer *et al.*, Phys. Rev. 126, 1710 (1962).

 $m^* = 2m_0$ , a value found both by Barker<sup>17</sup> and by Freder-<br>ikse *et al.*<sup>18</sup> The coupling constants—calculated by ikse *et al.*<sup>18</sup> The coupling constants—calculated by Eagles"—are now as follows:

$$
LO1-mode \alpha_1 = 1.83 \ (m^*/m)^{1/2} = 2.6
$$
  

$$
LO2-mode \alpha_2 = 0.50 \ (m^*/m)^{1/2} = 0.7.
$$

The corresponding polaron mass is  $\lceil \text{Eq.} (2) \rceil$ :

$$
m_P = 2.0 \left( 1 + \frac{2.6 + 0.7}{6} \right) m_0 = 3.1 m_0.
$$

The mobilities computed from Eq. (1) are plotted in Fig. 2. The agreement is reasonable; above room temperature, the theoretical values deviate at most  $40-50\%$ from the experimental data points.

Some of the values chosen for the parameters in Eq. (1) as well as the evaluation of  $\mu$  are subject to question. One can argue that  $m_{\text{eff}}=2m_0$  is the value of the polaron mass. Hence the real "bare" mass is about 1.5  $m_0$  and the  $\alpha$ 's are 10 to 20% smaller. This would increase the calculated mobilities slightly. However, the reasonable agreement with experimental data would not alter drastically. It is also legitimate to raise objections concerning the evaluation of  $\mu_{\text{tot}}$  by adding  $\mu_1$  and  $\mu_2$ reciprocally. This procedure is a not completely justifiable extrapolation from the weak coupling range. However, considering that very little is known about the interaction of the two scattering processes (the  $LO<sub>3</sub>$ and the  $LO<sub>2</sub>$  mode), and taking into account that the coupling constants are not too far removed from the perturbation range, the assumption of independent scattering by the two modes is not unreasonable.

#### B. Low-Temperature Range  $(T<10^{\circ} K)$

Table I lists values of the Hall mobilities of several doped and reduced samples at 4.2'K. These mobilities depend strongly on the impurity concentration  $N$ ; the temperature dependence between 1 and 10'K is very small (see Fig.  $1$ ). Because all carriers are in the conduction band, and because the donors from which these carriers originate are the dominant impurities,  $N$  is related in a simple way to the charge-carrier concentration  $n$ . In the case of Nb and La doping, there is strong evidence that these ions substitute for Ti<sup>4+</sup> and Sr<sup>2+</sup>, respectively.<sup>20</sup> Hence the donor charge is  $1+$ . Recent publications suggest that the donor in reduced Recent publications suggest that the donor in reduced<br>SrTiO<sub>3</sub> is an oxygen vacancy.<sup>21</sup> The fact that the Hal coefficient does not change up to  $1000^{\circ}$ K would indi-

<sup>18</sup> H. P. R. Frederikse, W. R. Thurber, W. R. Hosler, J.



FIG. 2. Hall mobility of electrons in  $SrTiO<sub>3</sub>$  above 200°K. The solid line represents calculated values using Eq. (1). Measured mobilities are labeled as follows:  $\bullet$  La  $2:0.1\%$  La,  $\bigcirc$  La  $3:0.025\%$ La,  $\times$  Nb 5:0.05% Nb,  $\Box$  Nb 15: 0.01% Nb

cate that these donors are already completely ionized at 1'K and that the charge is 2+.

The dependence of the mobility at  $4.2^{\circ}\text{K}$  on carrier concentration  $({\sim}Z$  times impurity concentration) is presented in Fig. 3. The data lie approximately on two straight lines (dashed): an upper one for doped specimens and a lower one (smaller by a factor 3.5-4.5) for reduced samples. Both lines show that  $\mu \propto n^{-x}$ , where  $x=0.85\pm0.03$  for the doped specimens, and  $x=0.75$  $\pm 0.03$  for the reduced ones.

There are two extrinsic collision processes that depend on the concentration of impurities: neutral and ionized impurity scattering. The fact that for most of the samples investigated the number of (charged) donors



FIG. 3. Mobilities at  $4.2^{\circ}$ K of reduced and doped samples as a function of carrier concentration. The dashed lines are drawn as an average of the experimental values. The solid lines show the results of theoretical predictions [Eqs.  $(9)$ ,  $(10)$ , and  $(11)$ ].

<sup>&</sup>lt;sup>17</sup> A. S. Barker, in *Proceedings of the International Colloquium on*<br>Optical Properties and Electronic Structure of Metals and Alloys,<br>Paris, 1965 (North-Holland Publishing Company, Amsterdam, 1965).

Babiskin, and P. Siebenmann, Phys. Rev. (to be published).<br><sup>19</sup> D. M. Eagles, J. Phys. Chem. Solids 26, 672 (1965).<br><sup>20</sup> Osamu Saburi, J. Phys. Soc. Japan 14, 1159 (1959).<br><sup>21</sup> A. E. Paladino, L. G. Rubin, and J. S. Waugh, Solids 26, 391 (1965).

introduced by doping or reduction is considerably larger than the concentration-of existing (neutral) iona or imperfections removes the neutral impurity scattering as a major process. Ionized impurity scattering has been treated theoretically by Conwell and Weisskopf<sup>22</sup> and treated theoretically by Conwell and Weisskopf<sup>22</sup> and<br>by Brooks and Herring.<sup>23</sup> The first two authors calculated the collision cross section in the Coulomb field on the basis of small scattering angles. The latter pair used a screened Coulomb potential and the Born approximation. Both assumptions can be described by the condition  $ka \gg 1$ , (4)

$$
ka \gg 1,\tag{4}
$$

where  $k$ = wave vector, and  $\alpha$ = screening radius. At low temperatures,  $k(=k_F)$  is of the order of several times  $10^6$  cm<sup>-1</sup>, while a is about 3-10 Å (calculated for SrTiO<sub>3</sub> containing  $7 \times 10^{18}$  carriers/cm<sup>3</sup>; see below). Hence the product  $ka$  has values between 0.2 and 0.6 and the condition (4) is not valid. In other words, the electron energy is small compared with some measure of the scattering potential and the Born approximation is inapplicable.

The case  $ka \ll 1$  has been investigated by several au-The case  $ka \ll 1$  has been investigated by several authors including Sclar,<sup>24</sup> Csavinsky,<sup>25</sup> and Gulyaev,<sup>26</sup> all using the partial-wave technique. In this paper we will follow the Gulyaev treatment.

To start with, one assumes that the electron "sees" an interaction potential

$$
V(r) = \frac{Ze^2}{\epsilon} \frac{\exp(-r/a)}{r},
$$
 (5)

where  $Ze =$  impurity charge, and  $\epsilon$  = dielectric constant. The relaxation time of the collision process is given by

$$
1/\tau = N_i v \sigma_T, \tag{6}
$$

with  $N_i$ =number of scatterers, v=electron velocity  $(=v_F, \frac{1}{2}mv_F^2=E_F)$ , and  $\sigma_T$ =total scattering cross section. According to the partial-wave method,<sup>25,26</sup> if  $ka \lt 1$ , one can neglect all but the s-wave  $(l=0)$ phase shift and hence

$$
\sigma_T = \frac{4\pi}{k^2} \sin^2 \delta_0 = \frac{4\pi}{k^2} \frac{1}{1 + \cot^2 \delta_0}.
$$
 (7)

Using a variational principle, he derives the following formula:  $2.2 + 20$ <sub>2/3</sub> + 22

$$
\cot \delta_0 = -\frac{1}{4ka} \frac{\gamma a^2 + 2\gamma a + 32}{\gamma^2 a^2 + 8\gamma a},\tag{8}
$$

where

$$
\gamma = \frac{2m_D^*}{\hbar^2} \times \frac{Ze^2}{\epsilon}
$$

22 E. Conwell and V. F. Weisskopf, Phys. Rev. 77, 388 (1950).<br>
23 H. Brooks, Phys. Rev. 83, 879 (1951).<br>
24 N. Sclar, Phys. Rev. 104, 1548 (1956).

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- 25 P. Csavinsky, Phys. Rev. 126, 1436 (1962); 131, 2033 (1963);
- 135, AB3 (1964).<br>- 26 Yu V. Gulyaev, Fiz. Tver. Tela 1, 422 (1959) [Englis<br>transl.: Soviet Phys.—Solid State 1, 381 (1959)].

and  $m_D =$  density-of-states effective mass = 5  $m_0$ . Hence,

$$
\frac{1}{\tau} = 4\pi N_i v_F a^2 \frac{16(\gamma^2 a^2 + 8\gamma a)}{(\gamma^2 a^2 + 20\gamma a + 32)},
$$
\n(9)

from which one can easily calculate the mobility

$$
\mu = e\tau / m_M^*,\tag{10}
$$

where  $m_M^*$ = mobility-effective mass. Equations (9) and (10) show that the mobility is largely determined by the number of impurities, the velocity of the electrons and the screening length. The 6rst two quantities are unambiguous. The main question remaining is what to use for the screening length a. One can choose the Fermi-Thomas expression<sup>27</sup>

$$
a_F = \left(\frac{\epsilon}{4\pi e^2 N(E_F)}\right)^{1/2} = \left[\frac{\hbar^2 \epsilon}{4m_D e^2} \left(\frac{\pi}{3n}\right)^{1/3}\right]^{1/2}, \quad (11)
$$

where  $N(E_F)$  = density of states at the Fermi level, and  $n=$ electron concentration. Or one might prefer the Bohm-Pines screening length'

$$
a_B = \left(\frac{\hbar \omega_P{}^* \epsilon}{4\pi n e^2}\right)^{1/2} = \left(\frac{\hbar^2 \epsilon}{4\pi n e^2 m_M{}^*}\right)^{1/4},\tag{12}
$$

where  $\omega_P^*$  = plasma frequency. Using  $a_F$  for a in Eq. (9), where  $\omega_P^*$  = plasma frequency. Using  $a_F$  for a in Eq. (9) one finds  $\mu \sim n^{-1.0} f(\gamma a)$ , while substitution of  $a_B$  in the equation for  $\mu$  leads to  $\mu \sim n^{-0.83} f(\gamma a)$ . The factor  $f(\gamma a)$  contains the concentration n in such a way that it will decrease the power x in  $\mu \sim n^{-x}$ .

In order to obtain some perspective and to be able to judge the validity of the expressions (4) to (10), it is useful to calculate the values of some of the parameters for a particular value of  $n$ ;  $n=7\times10^{18}$  cm<sup>-3</sup> (sampl Nb 5).  $E_F = 3.6 \times 10^{-15}$  erg = 2.25 meV,  $k_F = 6 \times 10^6$  cm<sup>-1</sup>,  $v_F = 1.2 \times 10^6$  cm/sec,  $a = a_F = 2.3 \times 10^{-8}$  cm,  $a_B = 9.4$  $\times 10^{-8}$  cm,  $ka_F = 0.14$  or  $ka_B = 0.57$ , and  $\gamma = 1.5 \times 10^{+8}$ .  $cm<sup>-1</sup>$ . Two other quantities are of importance:

(a) the polaron radius $^{29,30}$ 

$$
r_P \approx \left(\frac{h^2}{2m\hbar\omega_l}\right)^{1/2} = 4.5 \times 10^{-8} \text{ cm for } \hbar\omega_l = 0.099 \text{ eV}
$$

$$
= 5.9 \times 10^{-8} \text{ cm for } \hbar\omega_l = 0.058 \text{ eV}
$$

and (b) the effective Bohr radius  $a^* = 1.25 \times 10^{-8}$  cm. The values of  $m<sub>D</sub>$  and  $\epsilon$  used for the calculation of  $a<sub>F</sub>$ were  $5m_0$  and 5, respectively; the latter is the value of the optical dielectric constant. A similar assumption was made for the calculation of  $a_B$ ; however, in this case,  $m_M^*$  is the mobility mass (=2m<sub>0</sub>). The choice of  $\epsilon = 5$ seems to be appropriate in face of the calculated value

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<sup>&</sup>lt;sup>27</sup> E.g., C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963), p. 112.<br><sup>28</sup> D. Bohm and D. Pines, Phys. Rev. 92, 609 (1953).<br><sup>29</sup> H. Fröhlich, Advan. Phys. 3, 325 (1954).<br><sup>29</sup> H. Haken in *Pol* 

and G. D. Whitfield (Plenum Press Inc. , New York, 1963), p. 269.

of the polaron radius; it means that at small distances from the impurity center the potential is rather large  $(\sim 1/\epsilon_{\rm opt})$ , but that at 4-6 Å the static value  $(\epsilon_{\rm stat})$  takes over, causing the potential to be negligible.<sup>30</sup> takes over, causing the potential to be negligible.<sup>30</sup> Hence, the value used for  $a$  in Eq. 9 must be smaller than  $r_p$ . This implies that the calculated value of  $a_F$  is probably all right, but that the figure for  $a_B$  is doubtful.

As a result of these considerations, the mobilities were computed using  $a=a_F$ . These values are shown as two solid lines in Fig. 3. The lower one, labeled  $Z=1$ , pertains to the Nb- and I.a-doped samples. It is clear that the theory underestimates the experimental mobilities by a factor of <sup>2</sup>—3. The upper line is calculated for  $Z=2$  and supposedly corresponds to the reduced samples (containing oxygen vacancies). Unfortunately the computed mobilities are somewhat higher than those for  $Z = 1$ , contrary to expectations. However, one should realize that the shape and strength of the scattering potential does not enter in  $N_i$ ,  $v$ , or  $a_F$ , but only in the "correction factor,"

$$
f(\gamma a) = \left[16(\gamma^2 a^2 + 8\gamma a)/(\gamma^2 a^2 + 20\gamma a + 32)\right],
$$

through the quantity  $\gamma$ . This correction factor does not depress the mobility enough to overcome the smaller number of scatterers when  $Z=2$   $(N_i=\frac{1}{2}\times \text{electron}$ concentration). In this case theory overestimates the experimental results <sup>2</sup>—4 times.

The discrepancy of a factor of <sup>2</sup>—4 between experimental and theoretical mobilities should not be taken too seriously. The choice of values for parameters like  $m^*$  and  $\epsilon$  is very difficult because it is not always clear if one should use the density-of-states mass, the "mobility" mass, or perhaps the transverse mass. Furthermore, for regions of the order of several atomic cells, there is good reason not to substitute  $\epsilon_{stat}$  for  $\epsilon$ , but rather  $\epsilon_{\rm opt}$ . On the other hand, at very small distances from the impurity center, the concept of a dielectric constant becomes altogether inapplicable.

#### C. Intermediate-Temperature Range  $(10-200)K$

A logical first attempt to fit the mobility in this temperature region is a simple, reciprocal addition of the extrapolated mobilities at high and at low temperatures. However, this procedure gives rise to values that are too high at all temperatures between 10 and 200'K and at 100'K by as much as a factor of 10.It seems that one or several, more effective, scattering mechanisms determine the mobility in the intermediate range. Yet, down to 90 or 100'K, there is very little spread in mobilities of samples of quite diferent electron concentration. Hence one should first explore intrinsic scattering processes. The third I.<sup>O</sup> branch of the phonon spectrum ( $\hbar \omega_{k} = 0.022$  eV) has a very small coupling constant  $\lceil \alpha(m/m^*)^{1/2} = 0.01$  according to Eagles<sup>31</sup>]. Consequently, its contribution to optical mode scattering is negligible. Another possibility is collisions with the acoustical modes. In this case one would expect a slight step in the mobility at the  $110^{\circ}$ K phase transition, because the elastic constants show a discontinuity of because the elastic constants show a discontinuity of several percent at this temperature.<sup>32</sup> However, careful and precise measurements of conductivity and Hall effect around  $110^{\circ}$ K have revealed no trace of a discontinuity.

One could consider scattering by the lowest transverse One could consider scattering by the lowest transvers<br>optical mode,<sup>10</sup> the "soft" mode.<sup>11</sup> Arguments agains such a process have been listed in the introduction of this paper.

We have explored all the intrinsic scattering mechanisms treated in the literature. Unfortunately, it has not produced a satisfactory explanation for the magnitude of the mobility in the intermediate-temperature range.

### **CONCLUSION**

The Hall mobility  $\mu_H$  of electrons in SrTiO<sub>3</sub> has been investigated between 1 and 1000'K. Above 300'K the temperature dependence and the magnitude indicate that longitudinal optical mode scattering is the limiting process. Order-of-magnitude agreementbetween theoretical predictions and experimental data implies that ionized impurity scattering is probably the major factor determining the mobility at very low temperatures (1–10°K). An evaluation of  $\mu$  using a cross section proportional to  $a_F^2$  (where  $a_F = \text{Fermi-Thomas screening}$ radius) yields values that are 2 to 3 times smaller than the experimental data for Nb- or La- doped specimens. This underestimation occurs in spite of the surprisingly small size of  $a_F$  (1.4 to 2.5 Å).

In comparing the theoretical and the measured values of the mobilities, it should be emphasized that both at high and at very low temperatures the *absolute* magnitude has been calculated without the use of any adjustable parameters.

At intermediate temperatures (10—200'K), another so far unknown collision process appears to contribute to the electron scattering.

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<sup>&</sup>lt;sup>31</sup> The value 0.001 for  $\alpha(m/m^*)^{1/2}$  in Ref. 19 is a misprint; it should read  $\alpha(m/m^*)^{1/2} = 0.01$ . D. M. Eagles (private communication)

<sup>3&#</sup>x27; R. O. Bell and G. Rupprecht, Phys. Rev. 129, 90 (1963).