Temperature dependence of the electron intersubband resonance on (100) Si surfaces

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The dependence of the electron intersubband resonance on temperature has been studied between 4.2 and 130 K for photon energies 10.45, 15.81, and 44.32 meV. At the highest energy, distinct transitions from the ground state to each of the next three higher-lying levels (i.e., the $0 \rightarrow 1$, $0 \rightarrow 2$, $0 \rightarrow 3$ resonances) are observed. With rising temperature, the lines originating from the 0 ground-state subband shift and diminish in amplitude. The effect is attributed to thermal population of the higher-lying levels, in particular the 0' subband of the fourfold degenerate valleys in the Si (100) surface. Firsthand evidence for the population of this level, and the existence of two distinct types of electrons at finite temperature, comes from the identification of a new resonance (i.e., the $0' \rightarrow 1'$ transition) which grows with increasing temperature.

I. INTRODUCTION

Intersubband resonance experiments have provided detailed information on the bound electronic states in a semiconductor surface space-charge layer. Experimental work is being pursued along three different lines—far-infrared absorption, ^{1,2} photoconductivity,³ and most recently, hot-electron induced far-infrared emission.⁴ The results have prompted concerted theoretical efforts to account for the many relevant physical features involved in the resonant excitation of the subband electrons.

The quantitative examination⁵ of the dielectric screening effect, as first suggested in Ref. 6, has given new emphasis to critical comparison of theory and experiment. The "satisfactory agreement" cited in papers of only a year ago has ceded to more searching analysis. Both dielectric screening and an exciton-like final-state interaction^{7,8} are part of the relevant physics. Ando^{8,9} calculates the position of the optical resonance, including image potential, exchange and correlation, dielectric screening and exciton effects. Vinter's perturbation calculation¹⁰ differs in that it ignores the final-state interaction in the subband resonance determination. The interaction, it is suggested, gives rise to a separate bound state and a second distinct resonance peak.

In effect, Ando's work shows the dielectric shift and exciton correction tend to cancel. Over the experimentally relevant range of electron density N_s the resonance energy does not differ significantly from the subband energy splitting for the 0 - 1 transition. This accounts for the reasonable agreement of the experimentally observed and calculated 0 - 1 energies in earlier work.² It also justifies the analysis in which subband energy splitting is approximately equated with resonance energy. According to Ando^{8,9} the difference between these two quantities is even less for the higher-order transitions $0 \rightarrow 2$, $0 \rightarrow 3$, etc.

The present experimental work extends the energy range of previous measurements to $\hbar\omega = 44.32$ meV, i.e., the 28- μ m line of the water-vapor laser. In Fig. 1 is shown the intersubband resonance spectrum for an inversion layer for various temperatures between 6 and 48 K. Under sweep conditions, for which the depletion charge is $N_{dep}^{*} = (1.1 \pm 0.1) \times 10^{11}$ cm⁻², the 0-1 transition is located at the surface electron density $N_s = (5.7 \pm 0.2) \times 10^{12}$ cm⁻² at the lowest temperature. As in previous



FIG. 1. Intersubband resonance for electrons in an inversion layer at various temperatures. At the high experimental photon energy of 44.32 meV, transitions from the ground state to the first, second, and third excited level are observed for the first time. Sample p-K1 has an oxide thickness of 2240 Å and a threshold of -0.5 V. dP/dV_g is the derivative optical power absorption and V_g the gate voltage.

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FIG. 2. Comparison of the experimentally determined resonance energies with recent calculations (T. Ando, Ref. 8). The experimental points are for Siemens metal-oxide-semiconductor capacitor samples under conditions where the depletion charge is 1.0×10^{11} cm⁻².

experiments² the threshold and effective depletion charge are determined from C-V curves taken along with the absorption spectrum. Figure 1 also shows transitions $0 \rightarrow 2$ and $0 \rightarrow 3$ for the inversion layer for the first time. Previous work at energies up to 15.81 meV had failed to show these because their resonance energy, even at $N_s \rightarrow 0$, exceeded the experimental $\hbar\omega$.

In Fig. 2 we show a comparison of observed and calculated resonance energies, that include the previously published² low-energy points. The values apply for low temperatures and a sample for which $N_{dep}^* = 1.0 \times 10^{11} \text{ cm}^{-2}$. The calculations, as supplied by Ando, are an extension to higher N_s of the work in Refs. 8 and 9.

The primary objective of this paper is to probe the temperature dependence of the spectra. Questions related to the thermal occupancy of various subband levels in the (100) Si surface are discussed in following sections of the paper.

II. RESULTS AND DISCUSSION

The temperature dependence is a straightforward extension of previously published work. Except for an additional sample heater and calibrated Ge thermometer, the apparatus is the same as previously described.² The experimental technique of charging the inversion layer in the presence of light, then removing the illumination and slowly sweeping to lower gate voltage (i.e., the "dark sweep" in Ref. 2), is also employed here. The samples are similar to those previously described. C-V curves are run concurrently to provide values of relevant parameters. The various effects—new resonance modes from thermally occupied levels, line shifts, amplitude variation with temperature, substrate bias effects, and the linewidth are discussed below.

A. New resonances

Raising the temperature will have the effect of thermally redistributing the electrons among the various surface subbands. We can expect to observe new resonance modes from thermally occupied levels, if the appropriate values of $\hbar\omega$ are used.

Figure 3 shows the 15.81-meV spectrum for a (100) Si inversion layer. At 11 K we reproduce the curve shown in previous work.² Raising T to 28 K causes a small extra peak to appear at low gate voltage V_g . As the amplitude (see inset) of the 0 - 1 transition decays, the new peak grows, until at 70 K the two peaks are about equal.

The only interpretation consistent with the known symmetry and subband structure of the (100) Si surface is that the new mode represents transitions from the thermally occupied lowest subband level



FIG. 3. Intersubband resonance at different temperatures for $\hbar\omega = 15.81$ meV. The inset shows the variation of the resonance amplitude for the $0 \rightarrow 1$ transition with temperature. Along with the decay of the $0 \rightarrow 1$ amplitude a new resonance from the thermally populated 0' level is observed.

of the fourfold degenerate valleys with light mass $(m_{ee}^* \sim 0.2m_0)$ normal to the surface. To distinguish these levels from the 0, 1, 2..., etc. subbands of the two heavy-mass valleys, they are labeled 0', 1', 2', etc. In these terms the new line is ascribed to $0' \rightarrow 1'$ transitions. Optical k-conserving transitions from the 0 to the 0' level are not allowed in the intersubband resonance experiments. Nevertheless, it is possible to infer something about this energy separation from the temperature dependence work. The data show substantial thermal occupation of 0' level at temperatures as low as 28 K and thus imply that 0' is quite close to the Fermi energy at $N_s = 1.4 \times 10^{11}$ cm⁻² where the resonance is observed. At finite temperature and low N_s a considerable fraction of the inversion layer electrons occupy the primed valleys. We explore this idea quantitatively in the adjoining discussion.

B. Amplitude variations with T

The amplitude of the 0 - 1 resonance reduces with rising T as indicated in the inset of Fig. 3. The linewidth remains remarkably constant to temperatures as high as 130 K4 Because the resonance energy does not exactly equal the subband separation, because matrix elements, many-body effects in the potential, dielectric screening, and final-state interaction are all temperature dependent, it is not a simple matter to relate the ob-



FIG. 4. Intersubband resonance at different temperatures for $\hbar\omega = 10.45$ meV.

served amplitude changes to a level spacing scheme. Nevertheless, the predominant effect that accounts for the amplitude decay in Fig. 3 is that electrons are thermally drained out of the 0 level. We proceed to describe the observed amplitude variation approximately according to the following simple scheme of a three-band model. We consider two-dimensional subbands 0, 1, and 0', with 0 and 1 separated according to the applied experimental energy $\hbar \omega$. The level 0' is assumed to have a density of states 4.3 times higher than 0 to account for the higher mass and degeneracy of the primed valleys. The Fermi energy and occupations n_0 , n_1 , n_0 , are calculated as a function of T using the unknown 0-0' spacing as a parameter. The resonance amplitude is assumed proportional to the occupation factor

$$(n_0 - n_1)/(n_0 + n_1 + n_0)$$
,

which in turn is compared with the experimental data. The energy separation 0-0' is chosen to get reasonable agreement with the experiments over a significant part of the *T* range.

Following this simple prescription we estimate levels 0 and 0' to be separated by 5 meV at the surface electron density, where the 0 - 1 resonance is observed in Fig. 3. The dotted line in the inset gives the expected amplitude variation. The many assumptions made in the description of the amplitude do not justify a more exacting comparison of the calculated and experimental results. The value 5 meV could be changed as much as ± 1 meV.

In Fig. 4, at the lower frequency of $\hbar\omega = 10.45$ meV, are shown data curves of the $0 \rightarrow 1$ resonance. The inset gives the amplitude variation. The amplitude decay occurs more rapidly than at the higher frequency. It is also described reasonably by assuming a 0-0' separation of 5 meV. The data in Fig. 4, where the $0 \rightarrow 1$ line is at $N_s = 2.0 \times 10^{11}$ cm⁻², allow an interesting comparison to the previously described $0' \rightarrow 1'$ line in Fig. 3. The latter occurs at $N_s = 1.4 \times 10^{11}$ cm⁻², not too different from the $0 \rightarrow 1$ line for 10.45 meV. We expect that the decay of the $0 \rightarrow 1$ resonance and growth of the $0' \rightarrow 1'$ line should description predicts that the $0' \rightarrow 1'$ line

$$n_0$$
, $/(n_0 + n_1 + n_0)$.

Allowing for the experimental difficulties in comparing amplitudes at two different frequencies, we have found that this is indeed the case. The growth of the 0' \rightarrow 1' line is described by a 0-0' spacing of 5 meV at $N_s = 1.4 \times 10^{11}$ cm⁻². In varying N_s from 1.4×10^{11} to 5.4×10^{11} cm⁻² a small rise the 0-0' separation would have been expected. The simple



FIG. 5. Effects of band-gap light on the intersubband resonance at different temperatures. The dashed line represents the experimental result at T=12 K without band-gap radiation. $I_{\rm LED}$ is the current applied to the light-emitting diode.

calculations that we have described are not sufficiently sensitive to show this effect clearly.

The 0'-1' resonance is not excited at $\hbar\omega = 10.45$ meV in Fig. 4, even though the 0' level is thermally populated. The energy separation 0'-1' exceeds the experimental $\hbar\omega$ at all values of N_s . At $\hbar\omega = 15.81$ meV the 0'-1' line is observed. It is again absent at the higher frequency $\hbar\omega = 44.32$ meV (up to $T \sim 50$ K in Fig. 1) because of the large 0-0' spacing and small fractional occupation of 0' at the N_s value, where the resonance is expected for this energy. With a further increase of N_s the resonance should reappear, even persist down to T = 0 K, as the 0' subband comes to lie below the Fermi energy. In general a delicate choice of $\hbar\omega$, T, and N_{dep}^* is required to observe the 0' - 1' line.

The use of band-gap light on the sample allows a check of our explanation for the missing 0' - 1'line in Fig. 4. Light, as shown previously, reduces the depletion charge. At the low temperature of 12 K in Fig. 5 it is seen to cause a considerable shift of the 0 - 1 line to higher gate voltage. The 0 - 2 transition can be observed in the new "flattened" surface potential well. For T = 37 K in the lower half of Fig. 5 the 0 - 1 shift is found to be very small, when light is applied. The tendency to shift upward in V_{e} is compensated in part by the effect of increased thermal population of the 0' level in the light-induced "flat" surface potential. Additional direct evidence for 0' population is the strong $0' \rightarrow 1'$ signal that is observed in the presence of light at $\hbar\omega = 10.45$ meV.

C. Accumulation layer resonances. Substrate bias experiments

The thermal occupancy of the 0' level is a function of level separation and hence depends on the depletion layer charge N_{dep}^* . In contrast to the previous inversion layer data (Figs. 1, 3, 4), the accumulation layer resonance represents the limiting case of vanishing depletion charge. The potential is primarily the self-consistent potential of the space-charge layer. In sweeping the gate voltage as in Fig. 6 at low T, one always achieves the resonance condition for $0 \rightarrow 2$, $0 \rightarrow 3$, etc. in addition to the $0 \rightarrow 1$ transition. In accord with the calculations⁹ the unresolved higher-order transitions appear as a broad precursor absorption.² Along with the higher-order lines from the un-



FIG. 6. Intersubband resonance in an accumulation layer for different temperatures. $\hbar\omega = 10.45$ meV. The scale of dP/dV_g is different for different temperatures. $V_{\rm FB}$ is the flat-band voltage.



FIG. 7. Substrate bias experiments at two different temperatures. V_0 marks the voltage, where the bias voltage sweep is started. The value of the depletion charge at the position of the resonance is as indicated. $N_s = (1/e)C_{ox}(V_0 - T_T); d_{ox} = 2240$ Å.

primed valleys one also achieves the resonance condition for 0' - 1' transitions regardless of the choice of $\hbar\omega$. The strong peak in Fig. 6, that grows with increasing temperature at low gate voltage, must be ascribed to a superposition of the possible resonances from the 0' to 1', 2', ... levels. The pronounced shift of the 0-1 line, along with the rapid decay of its amplitude, indicates considerable thermal redistribution of the charge in the surface subbands.

Accumulation represents the case of negligibly small depletion charge. We can, on the other hand, achieve an increase of this parameter for a given inversion layer sample by making use of the "bias sweep" technique.² This allows us to explore qualitatively the 0-0' separation with increasing N^*_{dep} . Figure 7 shows the results of such experiments.

On the left half of Fig. 7 are shown T = 70 K curves. At this temperature and $\hbar\omega = 15.81$ meV, the $0' \rightarrow 1'$ resonance is observed at low N_s value in a "dark sweep." If, as in a conventional "bias sweep," we start the gate voltage at a value V_0 below the $0' \rightarrow 1'$ line, the resonance is not observed at all (lowest trace, left half of Fig. 7). The interpretation of this fact is that the 0' carriers transfer back to the 0 level as N_{dep}^* is being raised in the course of the bias sweep.

This retransfer to the 0 level is also noted in the amplitude of the 0 - 1 line. At the low temperature of 16 K, as in the right half of Fig. 7, we observe the usual amplitude decay incurred in the "bias sweep" experiment because of the decreasing number of electrons in the surface layer, when V_0 is decreased. By way of contrast with this result, the 70-K curves show hardly any decrease of the amplitude as V_0 is lowered. The interpretation is that the effect of decreased total charge is made up by the increasingly higher fraction in the 0 level as the substrate bias is raised.

The lineshifts observed in the "substrate bias" sweep of Fig. 7 are additional evidence for this retransfer of 0' electrons to the 0 level. Without this effect at T = 16 K, the $0 \rightarrow 1$ line shifts to lower V_g . At 70 K we observe the opposite effect. The resonance moves in the direction of higher V_g . The downward substrate bias shift is counteracted by the upward shift caused by increased occupation of the 0 level (compare Sec. II D).

D. Lineshifts

A feature intimately connected with the thermal population of higher-lying, spatially more extended levels is the shift of the 0 + 1 resonance to low gate voltage. The effect for a given sample and N_{dep}^{*} becomes more noticeable with higher frequency (compare Figs. 1, 3, 4). Comparing the accumulation and inversion results at fixed frequency, we find the shift for accumulation (Fig. 5) to be stronger than for inversion (Fig. 4).

The self-consistent potential, the various manybody corrections to the potential, the dielectric screening, and the exciton effect are all expected to depend on temperature. It is probably a difficult matter to give a full account for all these effects. No calculation is presently available with which the observations can be compared quantitatively. Recently, Kamgar¹¹ has attributed the observed temperature-induced shift of the intersubband resonance for (111) Si electron accumulation layers to a reduction of the many-body interactions.

We can qualitatively explain the direction of the shift and the observations related to frequency and N_{dep}^* in terms of the self-consistency aspect of the surface potential only. As considered in the work of Stern,¹² the effect of thermal occupancy of the 0' level is to spread out the charge. The applied electric field is therefore screened less in the region where the 0 and 1 states are confined. The 0-1 energy splitting increases at fixed N_s , and thus implies a downward shift of the resonance at fixed $\hbar\omega$. This simple argument gives correctly the sign of the shift.

It also follows that the temperature-induced shift will be increasingly more important with rising $\hbar\omega$ and N_s . Self-consistency of the potential becomes an important feature with $N_s \ge N_{dep}^*$. In the limit $N_{dep}^* \gg N_s$ thermal redistribution of the charge among the surface subbands will not affect the level spacings.

E. Lifetime effects

The width of the optical resonance is expected to relate to the lifetime of the electronic states involved in the transition. We estimate a lifetime according to

 $\mathcal{T}=2\hbar/\Delta E,$

with ΔE obtained from the measured maximum to minimum separation of the absorption derivative signal and the E_{10} vs. N_s curve (Fig. 2).

The present work covers for the first time a sufficiently wide range of N_s values to allow the observation of a maximum in T vs. N_s . As in previously published work,^{1,2} we find T to increase with N_s and $\hbar\omega$ up to 15.81 meV. The newly observed 44.32-meV resonance (Fig. 1) shows a distinct reduction of T at high N_s . This allows us to conclude that there exists a maximum value of τ at some intermediate N_s . In this respect the intersubband resonance lifetime resembles the lifetime determined from transport experiments on similar samples.¹³ We do not observe any significant dependence of lifetime on T. The observed linewidths are essentially independent of temperature up to 130 K. It appears that phonon scattering is not observable in the intersubband resonance. This result is unexpected and differs from observations on the dc conductivity and cyclotron resonance for similar samples. The work of Kübleck and Kotthause¹⁴ permits a direct comparison. The low temperature w T value for cyclotron resonance on a sample from the same disc as p-K1 was found as $\mathcal{WT} = 6$ at $N_s = 5 \times 10^{11}$ cm⁻². It can be compared directly with the sample used in the work of Ref. 13, where a decrease of \mathcal{T} by a factor 3.3 up to T = 65 K is found. At the same density N, the 'resonance line $0 \rightarrow 1$ in Fig. 3 broadens by less than 10% up to T = 130 K!

III. CONCLUDING REMARKS AND DISCUSSION

Throughout the paper we have discussed and interpreted the results with reference to the conventional description of the Si (100) surface subband structure, i.e., a two-fold degenerate 0, 1, 2, ..., etc. system of subbands, separated in energy from a higher-lying four-fold degenerate primed subband ladder 0', 1', 2', etc. The primed levels are located close to the Brillouin zone boundary, whereas the unprimed levels lie at the zone center. Direct optical transitions are forbidden between the two systems of subbands.

This model serves well to explain qualitatively all the many observations related to the appearance of the new resonance mode and the amplitude decay of the 0 - 1 line. A point in question is the value of the relative energy separation of the two subband ladders, i.e., the 0-0' energy spacing. We have given an approximate analysis of the amplitude decay with many simplifying assumptions and have found a 0-0' separation of about 5 meV for $N_{\rm s}$ in the range $2 \times 10^{11} - 5 \times 10^{11}$ cm⁻² and a depletion charge $N_{dep}^* = 1.1 \times 10^{11} \text{ cm}^{-2}$. The values that have been found are smaller than a simple estimate would lead us to expect. The 0-0' separation for this N_{dep}^* and N_s has not been calculated, and we proceed to estimate it as follows. The $0 \rightarrow 1$ resonance occurs at 10.45 meV at $N_s = 2.0 \times 10^{11}$ cm⁻². Ando⁸ gives the energy separation as ~15% higher for this case, i.e., ~12 meV. If we scale the 0-1 energy according to the triangular potential well prescription (a factor of about 0.9), we arrive at a 0-0' separation of ~11 meV. At $N_s = 5.0$ $\times 10^{11}$ cm⁻² the separation would be even larger. The simple experimental fact that the 0'-1' resonance is observed already at less than 30 K argues convincingly that the 0' level must lie closer than this estimate. There is a distinct discrepancy here.

A second point to consider is the energy of the 0'-1' resonance as observed at $N_s = 1.4 \times 10^{11}$ cm⁻². Interpolating the experimental points for the 0+1 resonance, we estimate that at this value of N_s it would require an energy of 9.5 meV. The triangular potential predicts a scaling factor of 1.7 between the 0'+1' and 0+1 resonances. We expect the 0'+1' resonance at ~16.0 meV, to be compared with the 15.81 meV of the laser line. We conclude that there is satisfactory agreement.

The only discrepancy that we encounter in the interpretation, it appears to us, concerns the numerical value of the 0-0' energy separation. One possible explanation for the smaller observed value is interface grading.¹⁵ Another is the existence of a uniaxial surface strain. If the stress were directed along a [100] direction, it would remove the four-fold degeneracy of the 0' level. The analysis in Sec. II B would have to be changed accordingly.

If, however, we view the present results in relation to the cyclotron resonance work in Ref. 14, there appears a genuine problem. The cyclotron mass in the 0 subband is $\sim 0.2m_0$, that in the 0' level $\sim 0.4m_0$. One observes in cyclotron resonance, when there is thermally-induced partial occupation of the 0' subband, only a single resonance line with mass value intermediate to those of the two-valley systems. There are not observed two cyclotron lines, as the present considerations of 0 and 0' occupation and the observation of two distinct intersubband resonances would lead one to expect. The partial occupation of the 0' level induced by uniaxial stress also results in a behavior of the surface conductivity¹⁶ and cyclotron

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resonance¹⁷ that is characteristic of only one group of electrons.

There is as yet no way out of this dilemma, but the recent work of Kelly and Falicov¹⁸ may point in the right direction. The theory considers intervalley coupling in a charge density wave state. The cyclotron mass is that of the interacting electron system. The intersubband resonances would have to be interpreted as two modes of the coupled valley subbands. This description may provide an answer for why the new, thermally occupied level appears closer to the ground state than one had expected. It remains, however, to show that such a theory of the surface levels can account equally well for all the many other features that have been observed and discussed in this work.

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- ¹A. Kamgar, P. Kneschaurek, G. Dorda, and J. F. Koch, Phys. Rev. Lett. 32, 1251 (1974).
- ²P. Kneschaurek, A. Kamgar, and J. F. Koch, Phys. Rev. B 14, 1610 (1976).
- ³R. G. Wheeler and H. S. Goldberg, IEEE Trans. Electron Devices 22, 1001 (1975).
- ⁴E. Gornik and D. C. Tsui, Phys. Rev. Lett. <u>37</u>, 1425 (1976).
- ⁵S. J. Allen, D. C. Tsui, and B. Vinter, Solid State Commun. 20, 425 (1976).
- ⁶W. P. Chen, Y. J. Chen, and E. Burstein, Surf. Sci. <u>58</u>, 263 (1976).
- ⁷B. Vinter, Phys. Rev. Lett. <u>35</u>, 598 (1975).

- ⁸T. Ando, Solid State Commun. <u>21</u>, 133 (1976).
- ⁹T. Ando, Z. Phys. (to be published).
- ¹⁰B. Vinter, Phys. Rev. B <u>15</u>, 3947 (1977).
- ¹¹A. Kamgar (unpublished).
- ¹²F. Stern, Phys. Rev. B <u>5</u>, 4891 (1972).
- ¹³G. Abstreiter, J. P. Kotthaus, J. F. Koch, and
- G. Dorda, Phys. Rev. B 14, 2480 (1976).
- ¹⁴H. Küblbeck and J. P. Kotthaus, Phys. Rev. Lett. <u>35</u>, 1019 (1975).
- ¹⁵F. Stern, Solid State Commun. <u>21</u>, 163 (1977).
- ¹⁶I. Eisele, H. Gesch, and G. Dorda, Solid State Commun. <u>18</u>, 743 (1976).
- ¹⁷P. Stallhofer, J. P. Kotthaus, and J. F. Koch, Solid State Commun. <u>20</u>, 519 (1976).
- ¹⁸M. J. Kelly and L. M. Falicov, Phys. Rev. Lett. <u>37</u>, 1021 (1976).