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INFRARED ABSORPTION SPECTRUM OF FREE CARRIERS IN POLAR SEMICONDUCTORS

Progress Report

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B. Jensen

Boston University

Boston, Massachusetts

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NOTICE

Abstract

The Drude Zener theory of the absorption of high frequency radiation by free carriers (inverse bremsstrahlung) has been extended into the quantum region ($\hbar w > k_o T$) in terms of a frequency dependent relaxation time which predicts the dc mobility in the quasiclassical limit. Numerical calculations of the frequency and concentration dependent electron scattering rate have been completed for InP, InAs, $Ga_{0.47}In_{0.53}As$, and previous results for GaAs extended to high carrier concentrations. When starting from a quantum statistical theory, the fact that $n_q^o \hbar w \rightarrow k_o T$ at low frequencies can be used to prevent the divergence of the coulomb scattering rate without inclusion of a screening radius. A result containing no adjustable parameters is found which predicts a mobility for uncompensated samples that decreases strongly at high concentrations. This has been observed in GaAs, and is not accounted for by the usual dc calculation which assumes $\hbar w = o$ and a screening parameter. Calculated results for GaAs are in good agreement with experimental measurements of the mobility which are found to be independent of a wide variety of conditions of material preparation. This indicates that disagreement with previous theoretical calculations was not due to compensation.

Calculations for ZnSe and further investigation of the modification of the optical constants by the presence of an intense laser field and by a static magnetic field are currently planned.

The classical Drude Zener theory for the transfer of energy from a high frequency radiation field to joule heating in a solid through free carrier absorption is known, from experimental measurements of the optical properties of semi-conductors, to require a quantum mechanical extension in the near infrared.[(1)-(11)] This occurs because of a breakdown at these frequencies of the conditions required for the validity of the quasiclassical Boltzmann transport equation from which the Drude Zener theory follows. (An extensive discussion is given in the enclosed preprint and hence will be omitted here.)

A high frequency extension of the Drude Zener theory for free carriers in polar semiconductors has been derived from a quantum extension of the Boltzmann transport equation.[(12)] Results are obtained in terms of a frequency dependent relaxation time which reduces to the quasiclassical limit at low frequencies for elastic scattering mechanisms, and gives the quantum result at high frequencies when used in the Drude Zener formula for the optical conductivity.[(13)-(17)] Inelastic polar optical mode scattering, charged impurity scattering and deformation coupled acoustic mode scattering are considered. Extensive numerical results have been calculated for the frequency and concentration dependent scattering rates for a number of compound semiconductors and comparison made with available experimental data. Previous calculations for light to moderately doped GaAs have been extended to include materials of very high carrier concentrations and an analysis has been made of the role of screening in coulomb scattering, which determines the mobility at high carrier concentrations and is the source of numerical differences between various theoretical calculations. The temperature dependence of the electron scattering rate and mobility have been examined. When used to predict the dc mobility as a function of concentration, the low frequency limit gives good results for InAs, InP, and $G^{a}As$. Reasonable results are also obtained for the ternary compound $Ga_{0.47}In_{0.53}As$.

A simple analytical expression for the low frequency Drude limit of the charged impurity scattering rate at high concentrations is derived which gives a good approximation to the exact result which must be integrated numerically.(12) Because one starts with a quantum statistical theory, the fact that $n_q^o \hbar w \to k_o T$ at low frequencies (where $\hbar w$ is the photon energy and n_q^o the equilibrium photon occupation number) can be used to prevent the divergence of the coulomb scattering rate without inclusion of a screening radius. A result which contains no adjustable parameters is found. The calculated mobility for uncompensated samples then shows a strong decrease at high concentrations which the usual dc calculation, which assumes $\hbar w = 0$ and includes a screening parameter, fails to predict. This has been observed experimentally in GaAs. Calculated results for GaAs at 77°K are in good agreement with experimental measurements of the mobility at this temperature which were found to be independent of a wide variety of conditions of material preparation. This indicated that the disagreement with previous theoretical results was not due to compensation, as had originally been postulated.

Numerical calculations of the frequency and concentration dependent electron scattering rate have been completed for InP, InAs, $Ga_{0.47}In_{0.53}As$ and previous results for GaAs extended to high doped materials. It was found that the theory could be applied to ternary compounds where alloy scattering is unimportant, and hence possibly to quaternary compounds. It is hoped to extend investigations to these materials in the future. The optical constants for InP and InAs have been calculated. Calculations for ZnSe will begin shortly.

For the coming year, the main emphasis in the theoretical program will be on further investigation of the effect on the electron scattering rate of an intense laser field and also of a static magnetic field.

In the case of the high intensity laser field, the formulation of the quantum extension of the Drude Zener theory enables one to consider the non-linear effects in terms of a field dependence of the scattering rate at high fields. The joule heating is given by the carrier concentration times the energy increase per electron in the presence of the field times the scattering rate.[12] If the intensity is low, the scattering rate is calculated using the unperturbed wave functions and electron energies of the solid which are known from the Kane theory.[18] If the intensity is high, the wave functions and electron energies become functions of the field[19] and the correction to the electron energy is $e^2E^2/2m_n w^2 = e^2A^2/2m_n c^2$. If this is not negligible, compared with the unperturbed electron energy e_k, the scattering rate becomes a function of E^2 just as it becomes a function of w when the photon energy is not negligible compared with e_k and the final electron state is given after scattering and photon absorption by $e_k + \hbar w$.

In the case of the magnetic field an analogous statement holds. The presence of the magnetic field modifies the electron energy levels and wave functions introducing the dependence on H. The modification of the wave functions in this case can introduce considerable mathematical complications. An indication of this can be seen from Ref. (20) where one does not have the additional factor of bandstructure. One can shown that the matrix elements for the second order transition with $\vec{E}$ perpendicular to the magnetic field are multiplied by an exponentially decreasing factor, while the free carrier absorption for $\vec{E}$ directed along the field is unchanged except for reduction by a factor of ½. However, the physical results tend to be obscured by the mathematical formulation and it is felt that this should be subject to simplification for the following reason. One can show that the quantity corresponding to $e^2E^2/2m_nw^2$ in the case of the laser field is $L^2/2I = /hw_c(n + \frac{1}{2})$ where $L = Iw_c$ is the angular momentum of the orbit, w_c is the cyclotron frequency, and $I = m_nr^2$, where r is the quantized radius of the orbit perpendicular to the magnetic field. The rotational kinetic energy must be large compared with k_oT and one requires $w_ct > 1$, so that the orbital period is small compared with the scattering time. One can see that the case where $L^2/2I = /hw_c(n + \frac{1}{2})$ is large corresponds to high fields or large quantum numbers, and the latter case is the classical limit, in which simplification should be possible.

A continuing investigation of the conductivity in the presence of an intense laser field, including nonlinear effects on the electron scattering rate, is planned for the coming year, in addition to the calculation of the frequency and concentration dependence of the scattering rate for ZnSe.

Work on the quantum theory of magnetoconductivity, including an investigation of the approach to the classical limit as discussed above, would be a continuing project, extending to a third contract year. We hope to have developed an analytical treatment, capable of the prediction of numerical results, for comparison with experiment by the end of the third year.

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PUBLICATION LIST OF PRINCIPAL INVESTIGATOR

1. "The Quantum Mechanical Extension of the Drude Zener Theory in Polar Semiconductors," B. Jensen, to be published.

2. "The Frequency Dependent Relaxation Time of Free Carriers in InP," B. Jensen, Journal of Applied Physics 50, 5800 (1979).

3. "The Infrared Absorption Spectrum of n-Type GaAs," B. Jensen, Physica Status Solidi B, 86, 291 (1978).

4. "The Optical Conductivity of Free Carriers in GaAs," B. Jensen, Solid State Communications 24, 853 (1977).

5. "The Quantum Mechanical Extension of the Boltzmann Transport Equation and Optical Absorption in Semiconductors," B. Jensen, Annals of Physics, 95, 229 (1975).

6. "Free Carrier Absorption in n-Type CdTe," B. Jensen, Journal of the Physics and Chemistry of Solids 34, 2235 (1973).

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A-II(a) - REIMBURSABLE OR COST-SHARING PORTION

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Prindipal Investigator, B. Jensen, Assistant Professor - 50% of time for academic year	9,250
100% of time for 2 summer monthes	3,560
1 Graduate Assistant 8 months 50% at 525/month=4200	4,200
Support Personnel	
Secretary - 1/8 of time	1,070
	18,080
2. Publications	3,200
3. Travel	1,800
Domestic: APS Meeting, APS divisional meeting (Solid State), APS divisional meeting (Plasma Physics)	
4. Other	
Computer Services	1,900
Fringe Benefits, 21% of Principal Investigator, 17% of secretarial	2,870
Total Direct Cost	27,850
5. Indirect Costs	
52.3% x total direct cost	14,570
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Principal Investigator B. Jensen
25% of time for 9 months - Academic Year.

A-II(a) - REIMBURSABLE OR COST-SHARING PORTION

1. Salaries and Wages

Scientific Discipline Personnel

Principal Investigator, B. Jensen, Assistant Professor - 50% of time for academic year	10,000
100% of time for 2 summer monthes	3,850
1 Graduate Assistant 8 months 50% at 560/month=	4,500

Support Personnel

Secretary - 1/8 of time	1,150
	19,500
2. Publications	3,300
3. Travel	1,900
Domestic: APS Meeting, APS divisional meeting (Solid State), APS divisional meeting (Plasma Physics)	
4. Other	
Computer Services	1,800
Fringe Benefits, 21% of Principal Investigator, 17% of secretarial	3,100
Total Direct Cost	29,600
5. Indirect Costs	
52.3% x total direct cost	15,480
	45,080

I It is requested that the Department of Energy provide 100% of the A-II(a) portion of $45,080.

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A-II(c) University Contribution of Principal Investigator

Principal Investigator B. Jensen
25% of time for 9 months - Academic Year.