Our research accomplishments under this contract cover a wide area of transport and electron-phonon interaction processes in artificially made semiconductor microstructures including a complete theory for picosecond relaxation phenomena and hot electron energy loss in semiconductor quantum wells and heterostructures, a theory for inelastic scattering in ballistic hot-electron transistors, a theory for elementary excitations in low dimensional semiconductor microstructures, a theory for the quasiparticle properties of semiconductor microstructures and a theory of bandgap renormalization. Our theory includes plasmon-phonon coupling, dynamical screening, ballistic transport, quantum wells, hot electrons, ultra small devices, energy...
Electron-Phonon Interaction and Transport in Artificially Made Semiconductor Microstructures

FINAL REPORT

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University of Maryland
Final Report for ARO Contract No. DAA29-85-K0233 (PI: S. Das Sarma)

Under our current ARO Contract (No. DAAG29-85-K0233) we have published (or have had accepted for publication) 68 papers in refereed journals in the last four years. In addition, there are about 10 papers which have either been submitted for publication or are under preparation. It is a reasonable expectation that we will have about 80 publications under the sponsorship of this contract. We have been invited to give about two dozen invited talks in major international conferences including the Hot Electron Conference (1987), APS March Meeting (1988), the Gordon Conference (1987), the Two-Dimensional Conference (1987), the Supertatlice and the Microstructure Conference (1987), the Ultrafast Phenomena Conference organized by the SPIE and the OSA (1988), various NATO Conferences (1990), International Device Conference (1989), etc. In addition, we have been invited to write a number of major review articles on "Electron-Phonon Interaction in Semiconductor Microstructures" by the World Scientific Press, by the Academic Press and by the Plenum Press. A list of the published papers and invited conference talks under the ARO contract is provided at the end of this section.

We also have produced four Ph.D.'s and six Masters' degrees on research done under the ARO Contract. Very recently, we have been asked to contribute a chapter on plasmon phonon coupling effects in ultrafast phenomena in semiconductor microstructures to a book on ultrafast processes being published by the Academic Press (edited by J. Shah of AT&T Bell Labs). This book (December 1990) will have articles by the leading researchers in this important subject area.

A significant feature of the work we have done under the current ARO contract is that most of the specific problems proposed by the Principal Investigator in the original ARO proposal (# 23220-EL) submitted in 1985 have been solved by during the three-year contract period. This includes fundamental and important issues such as picosecond hot carrier relaxation problem, dynamical screening and plasmon-phonon coupling effects in hot electron relaxation in III-V semiconductor
microstructures, slab modes and interface phonon effects in semiconductor microstructures, theory of polar scattering in heterojunctions and quantum wells, etc. Below we provide a very short description of the highlights of our specific research accomplishments under the ARO contract. The numbers in parenthesis after each subsection below refer to the publication list given at the end of this section.

1). **Hot electron relaxation in polar semiconductors.** We have developed a fairly complete quantitative theory for hot electron relaxation in polar semiconductors (both microstructural and bulk) within the electron temperature model. Our calculated results agree well with the measured energy loss rates\(^1\),\(^2\),\(^3\) in GaAs bulk\(^4\) and quantum well systems, both for steady-state electric field heating and photoexcitation experiments in the picosecond relaxation regime. Our theory includes hot phonon effect, quantum degeneracy, dynamical screening, plasmon-phonon and quasiparticle-LO phonon coupling effects. For quantum wells and heterostructures, it also includes electronic quantization (into subbands) and, very recently, phonon slab mode effects. Our theory gives a very good account of the experimentally measured electron energy loss rates to polar optical phonons, and, should have significant implications for device simulation in this regime. (Publication # 22, 24, 32, 34, 37, 40.)

2) **Self-energy effects in ultrafast processes.** In doing our research on the picosecond relaxation problem we have discovered that many-body coupling between quasiparticles and LO-phonons could lead to very significant effects on the hot electron transport properties. We find that quasiparticle renormalization of the bare LO-phonon mode leads to satellite LO-phonon peaks at quasiparticle energies. These quasiparticle-like LO-phonon excitations carry very little spectral weight (typically \(10^{-3} - 10^{-5}\) of the bare phonon mode) and are, under normal circumstances, not of any consequence. But, at low temperatures, they play
a very significant role in the hot electron relaxation process since these are the only LO-phonon modes that can be thermally occupied at low temperatures. Since thermal occupancy is an exponential process, it is clear that at some low temperatures, these novel quasiparticle-like LO-phonon modes are the main loss mechanism for the hot electrons in semiconductors. Our explicit detailed calculations bear out this simple physical picture and we think that we have identified an important "missing loss" mechanism\textsuperscript{15,16} at low temperatures which have earlier been mentioned in the literature. (Publication # 37, 40.)

3) **Polar scattering effects in microstructural transport properties.** We have calculated the polar scattering rate as a function of temperature, carrier density and the quantum well width in GaAs microstructures. The calculated results should be of direct relevance to the device simulation of high-speed modulation-doped field-effect transistors. (Publication # 15, 17, 26.)

4) **Ballistic hot-electron transistors.** We have done some preliminary calculations of inelastic mean-free paths in the ballistic hot-electron transistor (or, the hot-electron spectrometer) recently developed\textsuperscript{2} by the AT&T Bell Labs (Hayes and Levi) and the IBM (Heiblum) groups. Our calculation includes the dynamical screening and plasmon-phonon coupling effects on the electron-phonon interaction. (Publication # 12, 32.)

5) **Collective electronic effects in artificially structured materials.** We have investigated a number of different aspects of electronic collective modes in artificially made semiconductor microstructures. Perhaps the most interesting of these is our theory of plasmons in artificially made aperiodic (both quasiperiodic and random) multilayer structures. We showed that a study of plasmon dispersion and spectral weight via the light scattering Raman spectroscopy could be successfully used to study the important problem of Anderson localization. In particular, plasmons in Fibonacci and other quasiperiodic superlattices\textsuperscript{17} could,
in principle, show very interesting dispersion including Cantor set spectrum and fractal properties. We have also made a theoretical investigation of the magnetoexciton spectra of quasiperiodic semiconductor superlattices. Some of our theoretical predictions in this subject have already been verified experimentally. (Publication # 3, 10, 33.)

6) **Elementary excitation in semiconductor multiquantum well and superlattice systems.** We have developed a quantitative theory based on the RPA to describe the elementary excitation spectrum of quasi-two dimensional systems. In particular, the intra- and inter-subband excitations (both quasiparticle-like and collective) in quantum wells and multilayer structures have been calculated in details keeping the coupling between in-plane and out-of-plane excitations which is important at non-zero wavevectors. A specific and somewhat surprising finding is that the coupling between intra- and inter-subband excitations could have quite significant effect on the elementary excitation spectra of low dimensional structures. Our calculated spin-density and charge-density excitations are in excellent agreement with the available light scattering and infrared spectroscopic experimental results from the AT&T Bell Labs\textsuperscript{18}, the Max Planck Institute\textsuperscript{19} and the University of Hamburg\textsuperscript{20} groups. (Publication # 14, 16, 20, 31.)

7) **Electronic properties of quantum wire structures.** We were among the first groups to calculate the electronic structure of quasi-one dimensional quantum wires using a variational approximation. We have also obtained the elementary excitation spectra and the screening properties of quantum wire systems. We have also carried out a preliminary calculation of the optical properties of a lateral superlattice made with quantum wire arrays. This system is expected to be important in the next-generation infrared detection technology. (Publication # 8, 11, 13, 18, 28, 30.)
8) **Transport in quasi-one dimensional systems.** We have developed a quantum formalism to calculate the Drude transport properties of quasi-one dimensional semiconductor wires. Our theory which is based on the Kubo formula includes self-consistent level-broadening and screening, intersubband scattering and finite temperature effects. Our theoretical results are in reasonable agreement with the only available experimental results\(^7\) from the MIT JSEP program of Warren et al. carried out under the ARO sponsorship. Consistent with experiment, we find that at low temperatures and for high mobility samples, it should be possible to see quantum oscillations in the mobility of a quasi-one dimensional system. (Publication # 18, 30.)

9) **Fluctuating transport in mesoscopic systems.** We are one of the really active theory groups in this very exciting novel area of condensed matter physics.\(^10\) Phase coherence effects and lack of ensemble averaging lead to interesting fluctuations in low temperature transport properties of small systems (e.g. universal conductance fluctuation phenomenon, Aharonov-Bohm effect). We have carried out numerical simulation of such transport fluctuations in all three regimes of transport properties: Strongly localized variable-range-hopping regime; weak scattering, diffusive and weakly localized universal conductance fluctuation regime; and, the ballistic regime. We have numerically studied the transition from one to two-dimensional behavior in the variable-range-hopping transport fluctuations of small MOSFET's. Our results are in good agreement with the experimental results\(^21\) of the IBM group. We also predict a novel Aharonov-Bohm effect in the phonon-assisted variable-range-hopping transport of small highly disordered rings.\(^22\) We are also the first group to calculate universal conductance fluctuation results using the recursive Kubo formula. (Publication # 21, 27, 28, 29, 30, 41, 44, 45.)
10) **Vertical transport in superlattice minibands.** Very recently (basically in the last one year) experimental observation of carrier miniband transport along the superlattice growth direction (the so-called "vertical transport") has been reported by a number of groups\textsuperscript{23-25} using a variety of experimental techniques. Even though the currently available experimental data are preliminary, these are very exciting (and much more experimental results will be forthcoming in the near future) both from the fundamental electronic properties and device applications viewpoints. It may be worthwhile to point out that the original suggestion\textsuperscript{26} for the superlattice by Esaki and Tsu in 1969 was motivated by the possibility of interesting physics associated with vertical miniband transport.\textsuperscript{3} It has taken almost twenty years of advances in materials growth and fabrication techniques for us to be able to observe this phenomenon! Encouraged by these experimental results we have developed a quantum formalism (neglecting interference effects) to study miniband transport in superlattices. We find that the standard Bloch-Boltzmann picture of Drude transport breaks down in superlattice minibands since level broadening, temperature, chemical potential and the miniband width all have comparable energies and, therefore, the quasiparticle picture is invalid. Our numerical results are in excellent agreement with the experimental data.\textsuperscript{23} (Publication # 39.)

11) **Magnetic field effects on transport properties of microstructures.** Application of an external magnetic field has often led to new phenomena (e.g. Quantum Hall effect, Aharonov-Bohm effect) in microstructures. Equally important is the fact that experiments under an external magnetic field lead to a better understanding of the various scattering processes in microstructures. Motivated by various experimental results, we carried out a number of theoretical studies of magnetic field effects on transport properties. Notable among these is a study of the size quantization effect on the excitation gap in the fractional quantum Hall
effect. This work allowed for the first real quantitative comparison between theory and experiment in fractional quantum Hall effect and is used extensively by experimentalists. Earlier estimate of the excitation gap without the subband quantization effect was wrong by a factor of four! We also pointed out that the discrepancy between experiment and theory on magnetopolarons in GaInAs heterostructure is probably due to the role of interface phonon modes in the electron-phonon interaction. We also calculated the phase coherence length in two dimensions by solving the electron-phonon self-energy exactly and obtained detailed agreement with experiment in weak localization experiments. Finally, we calculated the transport and single-particle lifetimes in semiconductor microstructures and showed that in high-mobility modulation-doped systems, the transport lifetime could be larger than the single-particle lifetime by as much as two orders of magnitude! Thus even very high mobility structures could have lot of forward scattering and, thus, considerable broadening. Our theoretical predictions have been verified experimentally by the IBM group.27 (Publication # 5, 9, 21, 27, 29.)

12) Quantum tunneling. We have carried out very detailed theoretical calculations of the quantum tunneling problem in microstructures under high magnetic fields. As a first application of this theory we show that the quantum Hall effect could be affected in narrow quasi-one dimensional systems. This has already been verified experimentally. (Publication # 42, 43, 44, 45, 46.)

13) Resonant tunneling. We have developed a detailed theory for the elastic scattering effect on electronic resonant tunneling through the double-barrier-single-quantum-well structure. Such scattering could arise from either the ionized impurity scattering or the interface roughness scattering and has traditionally been discussed phenomenologically using a Breit-Wigner type formula. Our theory is in good agreement with existing experimental results and makes a
specific prediction about a novel type of electron focusing effect in resonant tunneling. (Publication # 58, 65.)

14) **Parabolic quantum wells.** We have carried out extensive electronic structure calculations of GaAs-Al$_x$Ga$_{1-x}$As parabolic quantum wells with a goal toward understanding their transport and optical properties. Our fully self-consistent numerical calculations include the effect of an external magnetic field and incorporates exchange-correlation corrections and the spatial variation of electron effective mass in such structures. The calculated results are in excellent agreement with the available transport and optical experiments. (Publication # 59.)

15) **Band-gap renormalization in quantum wells.** We have developed a detailed quantitative theory for the many-body band-gap renormalization in semiconductor quantum wells induced by electron-electron and electron-phonon interaction. Accurate quantitative information about band-gap renormalization is essential for the operation of many non-linear optoelectronic devices. Our theory shows that the band-gap renormalization in quantum wells is a universal function of dimensionless electron density and well width. Our calculated results are in excellent quantitative agreement with experimental results. (Publication # 51, 68.)

Even though we have done some other theoretical calculations (e.g. effect of impurity scattering on plasmon linewidths in semiconductors, a hydrodynamic theory of electronic linear response), the above items serve to provide an overview of our research accomplishments under the ARO contract. The technical details can be found in the actual publications, a list of which follows this paragraph. We believe that we have actually solved all the problems proposed in our original proposal No. 23220-EL submitted in 1985. We have shown an ability to attack the most important frontier problems in the subject and to come up with some
theoretical guidelines to understand the experimental results. A significant feature of our research is that it is inspired by experimental work and, in turn, our specific predictions have motivated a lot of experimental work. It is perhaps no surprise that our work is widely cited in the experimental literature.

Publications under the ARO Contract (published or accepted for publication):


50. Mobility Edge is a Model One Dimensional Potential (S. Das Sarma, S. He, and X.C. Xie), Phys. Rev. Lett. 61, 2144 (1988).


54. Calculated Shallow Donor-Level Binding Energies in GaAs-Ar\textsubscript{0.5}Ga\textsubscript{1.5}As Quantum Wells (M. Stopa and S. Das Sarma), Phys. Rev. B40, 8466 (1989).


Invited Talks in Major Conferences:

1. Invited Lecturer, "Elementary Excitations in Two Dimensions," 4th Canadian Summer Institute and Workshop on Theoretical Physics (Kingston, Ontario, Canada, Summer 1986).

2. Invited APS Symposium on "Inversion Layers with Lateral Constraints," (New York City, March 1987), Chair.


4. "Hot Electron Relaxation in Polar Semiconductors" (Invited Talk); 4th International Conference on Hot Carriers in Semiconductors (Boston, July 1987).
5. "Elementary Collective Excitations in Multilayered Two-Dimensional Systems" (Invited Review, with J. K. Jain); 7th International Conference on Electronic Properties of Two Dimensional Systems (Santa Fe, July 1987).


7. Invited Speaker, Workshop on High-Tc Superconductivity (University of Western Ontario, London, Canada, September 1987) "Possible Mechanisms for High-Tc Superconductivity".


11. Chair, Session on Silicon Epitaxy, APS March Meeting (New Orleans, March 1988).


13. Invited Speaker, International MMM and InterMag Conference (Vancouver, Canada, August 1988).


16. Invited Talk, Quantum Electrical Engineering Workshop of the Theoretical Physics Institute (Minnesota, October 1988); "Mobility Edge in a Model One Dimensional Potential."


18. Chair, Session on Quantum Hall Effect, APS March Meeting (St. Louis, March 1989).

19. Chair, Session on Many-Body Effects, APS March Meeting (St. Louis, March 1989).

20. Invited Speaker, Kathmandu Summer School on Theoretical Physics (Nepal, Summer 1989); "Unusual Solutions to the Usual Schrödinger's Equation."

22. Invited Talk, 36th Annual AVS Symposium (Boston, October 1989) "Non-equilibrium Crystal Growth".


24. Invited Plenary Lecturer, Brazilian Summer School on Low Dimensional Systems (Sao Carlos, Brazil, February 1990).

25. Invited Speaker, NATO Workshop on "Light Scattering in Semiconductors" (Canada, March 1990); "Excitations and Mode Coupling a Doped Polar System."


27. Chair, Session on Many-Body Theory, APS March Meeting (Anaheim, March 1990).

28. Chair, Session on Transport in Microstructures, APS March Meeting (Anaheim, March 1990).

29. Invited Speaker, NATO Workshop on "Transport in Microstructures" (Turkey, April 1990).

Ph.D’s granted under ARO sponsorship

1. X.C. Xie: "Fluctuating Transport in Microstructures" (June 1988).


4. Q. Li: "Elementary Excitations in Quasi-one Dimensional Quantum Wire Structures"

In addition six MS degrees in physics were granted to graduate students for research done under the ARO support.