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13. ABSTRACT (Maximum 200 words) Exciton and biexciton binding and excited state energies, and wave functions are calculated numerically via a finite element method in an effective mass approximation for GaAs quantum well disks and dots (including pyramid shaped structures) surrounded by an AlGaAs cladding. Moreover, the Al interdiffusion into the dot and the finite band offsets between the dot and the cladding have been included. For the range of dimensions studied, the inclusion of the Al interdiffusion had a pronounced effect on the binding energies when compared to those obtained from the infinite barrier model. Using the results of the exciton and biexciton calculation, we calculate the third-order nonlinear optical susceptibility as a function of pump-probe frequencies in a range about the exciton absorption resonance. We restricted our calculation to the optical nonlinearity via the biexciton state arising from the population saturation of the exciton state. We expect, depending upon dot dimensions, broadening parameter(s) size, and the amount of pump detuning, values of the imaginary parts of the susceptibilities to be on the order of -10^{-10} to -10^{-11} esu near resonance absorption due to biexciton formation.				
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EPSCoR Final Report
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**Excitonic Nonlinear Optical Properties
in Quantum Wires and Prismatic Dots**

Student: Robert O. Klepfer III
PI: Dr. Frank L. Madarasz
University: University of Alabama
in Huntsville

Grant No. F49620-92-J-0474
Parent Grant No. F49620-92-J-0382

Over the course of the grant, from September, 1992 through May, 1996, the student completed all academic requirements for a Ph.D., except a dissertation, including:

- Passed the departmental comprehensive exam required for admission to the Ph.D. program.
- Received a Master's degree in Physics from the above institution.
- Completed course work necessary for the Ph.D. program, maintaining a 3.8 GPA.
- Passed the physics department written qualifying examination.
- Wrote, presented, and successfully defended a thesis research proposal in accordance with physics department requirements and approval by the thesis committee which completed the requirements for the Ph.D. candidacy.
- Presently in the final stages of thesis research and has begun writing the dissertation.

In preparation for his research, the student:

- Learned FORTRAN and its application on the Alabama Supercomputer Network's Cray C94A super computer.
- Researched the literature to learn the state of technology in the areas of:
 - excitonic nonlinear properties in general
 - quantum confined structure fabrication and general properties
 - excitonic nonlinear properties of quantum confined structures
 - fabrication of InAs/GaAs triangular and tetrahedral dots in particular.

- Reviewed, under the tutelage of his advisor, basic principles of solid state physics, quantum mechanics, and point group theory.
- Communicated with Drs. Donald Dorsey and Kenneth Hopkins of the Materials Directorate at Wright Patterson AFB. Dr. Dorsey exchanged technical information with the student and sent the student his notes on the theory of epitaxy for the triangular quantum dot structure, helping to formulate the problem.
- Familiarized himself with the calculation and the code for the research performed under the parent grant and performed the final data runs with that code.
- Performed numerical computations for the parent grant research to include aluminum diffusion in the quantum wire structure.
- Defined the goals of the dissertation research, the motivation behind the research, and methods which will be utilized to accomplish the goals.

While working on his dissertation research, the student:

- Completed the "analytical" calculation of the exciton in a quantum disk, obtaining results which compare well to previous models reported in the literature for the ground state, as well as results depicting the higher states of the exciton.
- Attended the 1994 and 1995 March Meetings of the American Physical Society, at the latter of which he presented a paper detailing this first part of the calculation.
- Spent a considerable amount of time examining the literature on the Finite Element Method and, often through numerical experimentation, adapted this method of solving partial differential equations to quantum mechanical calculations.
- Wrote code to use the Finite Element Method to calculate the single particle states in 2D potential wells of any shape.
- Published one paper [Klepfer, Madarasz, and Szmulowicz, Phys. Rev. B **51**, 4633 (1995)] extending the original calculation of the parent grant to include another variational parameter, and submitted another, May, '96, to Physical Review B on "A dimensional parametric study of exciton/biexciton energies in rectangular GaAs/AlGaAs quantum well wires with and without finite band offset" with the same co-authors.

- Actively worked to establish a research network in his field and continues to interact with them.
- Extended the original code to take into account higher order elements in the finite element calculation. During the process of programming the original code, the student determined the code must use fifth order Hermite elements to be able to accurately model excitonic wave functions while keeping computation time within reasonable limits.

The student continues to write and refine the Finite Element Method code in order to include exciton and biexciton properties within various material systems. Since the student was awarded this grant quite early in his graduate career, incompleteness of the research by the termination date of the grant was foreseen, and a No Cost Extension was applied for and approved. During this no cost extension, the student was offered, and accepted, a position with Nichols Research Corporation. The position was not contingent upon completion of the degree, but a substantial incentive was applied to assure the student finishes his research and earns his degree. The student currently works at the University of Alabama in Tuscaloosa with full access to the tools he has used until now. He plans to defend his dissertation before the end of summer.