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This rpt contains a summary of significant accomplishments and progress during the reporting period. Programs to calculate pure crystal and alloy band structures have been completed and now include all important components, e.g. long-range interactions, spin-orbit interactions, and molecular CPA. The parameters that properly reproduce the band structures of light III-V compounds--GaP, InP, AlAs, GaAs, InAs, AlSb, GaSb, and InSb--have been selected and their band structures calculated. We are now prepared to run the band structures of the 14 three-component pseudo-binary alloys of these materials. These calculations were undertaken to test our procedures on a comparatively simple, well-characterized alloy system. The results agree with experiment and give satisfactory explanation of several features that were previously thought to be anomalous. It is clear that the general trends of the data and theory agree.

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SEMICONDUCTOR ENGINEERING  
FOR HIGH-SPEED DEVICES

Quarterly R&D Status Report 1

Covering the Period 1 June to 15 September 1985

18 September 1985

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MATTHEW J. KEEFER  
Chief, Technical Information Division

SRI International



## I DESCRIPTION OF PROGRESS

This report contains a summary of significant accomplishments and progress during the reporting period, 1 June to 15 September 1985.

Programs to calculate pure crystal and alloy band structures have been completed and now include all important components, e.g. long-range interactions, spin-orbit interactions, and molecular CPA.

The parameters that properly reproduce the band structures of light III-V compounds--GaP, InP, AlAs, GaAs, InAs, AlSb, GaSb, and InSb--have been selected and their band structures calculated. We are now prepared to run the band structures of the 14 three-component pseudo-binary alloys of these materials.

Two papers were published in this period and one other submitted on the  $\text{Si}_{1-x}\text{Ge}_x$  alloy:

- Krishnamurthy, S., A. Sher, and A.-B. Chen, 1985: "Generalized Brooks' Formula and the Electron Mobility in  $\text{Si}_x\text{Ge}_{1-x}$  Alloys," Appl. Phys. Lett., 47, p. 160.
- Krishnamurthy, S., A. Sher, and A.-B. Chen, 1985: "Binding Energy and Spectral Width of  $\text{Si}2p$  Core Excitons in  $\text{Si}_x\text{Ge}_{1-x}$  Alloys," Phys. Rev. Lett., 55, p. 320.
- Krishnamurthy, S., A. Sher, and A.-B. Chen, "Band Structures of  $\text{Si}_x\text{Ge}_{1-x}$  Alloys" (submitted to Phys. Rev. B).

These calculations were undertaken to test our procedures on a comparatively simple, well-characterized alloy system. The results agree with experiment and give satisfactory explanation of several features that were previously thought to be anomalous.

W.E. Spicer's group at Stanford is measuring the angle-resolved photo-emission spectra of  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  alloys, and we have calculated the energy and momentum dependent spectral density functions to compare with their data. Once again, this gives us a chance to compare the theory to a well-controlled experiment, although  $\text{HgCdTe}$ , a narrow gap semiconductor, lies outside the scope of materials we are to study under this contract. It is already clear that the general trends of the data and theory agree, but a detailed comparison must still be done. The result will be reported in the next period.



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We have started a literature search on various aspects of this program, e.g. hot electron theory and ballistic device analysis. One paper we have uncovered on hot electron theory looks particularly helpful\* In this paper, a technique is developed within the context of the many body Schrodinger equation to separate the center of mass and relative to the center of mass motions of electrons propagating through a medium in the presence of a strong electric field. The coupled center of mass and scattered motion equations are then solved in a kind of random phase approximation (RPA). RPA is a method of ignoring fast quantum coherence-induced transients and solving what amounts to a stationary state problem. Thus, RPA must be modified to treat the fast transient effects encountered in a ballistic transport device, but this approach should be more reasonable than those currently used, which depend on assumed drifted Maxwellian distributions.

## II EQUIPMENT PURCHASED OR CONSTRUCTED

None.

## III TRIPS, MEETINGS, PAPERS, AND VISITS

Papers published and submitted were listed in Section I. No other information to report in this area.

## IV PROBLEMS OR AREAS OF CONCERN

None.

## V DEVIATION FROM PLANNED EFFORT

None.

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\*Lei, X.L. and C.S. Ting, 1985: "Green's-Function Approach to Nonlinear Electronic Transport for an Electron-Impurity-Phonon System in a Strong Electric Field," Phys Rev. B32, p. 1112.

## VI FISCAL STATUS

As of this report, all work is progressing as scheduled. Contract dollars are \$611,296. To date, \$61,000 has been spent with \$80,000 available through 31 December 1985. Estimated date of completion is as scheduled.