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Dr. Peter A. Knipp

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Christopher Newport University
50 Shoe Lane
Newport News, VA 23606

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13. ABSTRACT *(Maximum 200 words)*

This technical performance report covers the FY-94 period. The principal investigator studied theoretically the optoelectronic properties of quantum wire and dot systems. These studies included lateral quantization in barrier-modulated wires, optical absorption by dots, and electron-phonon coupling in wells, wires, and dots.

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Performance Report for Grant Entitled "Optical and Transport Properties of Metallic and Semiconductor Nanostructures"

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Principal Investigator:

Dr. Peter A. Knipp

Department of Physics and Computer Science, Christopher Newport University

Newport News, VA 23606-2998

Phone: (804)594-7827

Fax: (804)594-7919

email: pknipp@pcs.cnu.edu

This technical performance report covers the FY-94 period. The principal investigator studied theoretically the optoelectronic properties of quantum wire and dot systems. These studies included lateral quantization in barrier-modulated wires, optical absorption by dots, and electron-phonon coupling in wells, wires, and dots.

I. INTRODUCTION

Semiconductor and metallic nanostructure systems are currently of great interest because of potential device applications such as solid-state lasers, optical modula-

tors, and single-electron switches. The properties of these materials are governed by fundamental excitations (e.g., phonons, electronic states, and photons) and by interactions between these excitations. Within nanostructures these excitations and their interactions figure prominently but often are significantly modified from their bulk counterparts. This has been seen for superlattices and quantum wells [1]. As fabrication techniques improve rapidly [2] it is important to consider such modifications for lower symmetry systems, such as quasi-one-dimensional or zero-dimensional heterostructures. The use of semimacroscopic models for calculating the excitations is very effective in these situations [3], yielding accurate predictions which either can be compared with experimental data in a diagnostic way or can be used to aid in the design of new nanostructures.

In FY-93 I worked on several aspects of the physics of quantum wires and dots. This work benefited from collaboration with scientists at the Naval Research Laboratory, particularly with Dr. T. L. Reinecke. Our current interests are optoelectronic properties of barrier-modulated structures and electron-phonon interactions in nanostructures. We have developed theoretical techniques for solving the nonseparable equations which govern fundamental excitations in these low-dimensional systems, and we have used these techniques to study the degree to which the systems' properties are modified by geometric factors. This work has born fruit in FY-93 and is ongoing. I will discuss barrier-modulated structures in Sec. II and electron-phonon interactions in Sec. III.

II. BARRIER MODULATED WIRES AND DOTS

This work involves collaboration with the experimental group of Professor A. Forchel at the Technical Physics Institute at the University of Wuerzburg (Germany). Dr. Reinecke and I do the theoretical work for this collaboration. The experimental

group has recently fabricated a novel type of semiconductor nanostructure, produced by lithography and etching of a GaAs barrier on top of a InGaAs quantum well which is on top of a substrate composed of either GaAs or AlGaAs. A diagram of the "barrier-modulated" wires and dots is shown as an inset to Fig. 1. In the case of wires, the advantage that this design has over others is that the wave function of the wire-localized carrier state is spatially separated from the etch-damaged semiconductor-vacuum interfaces which might otherwise provide nonradiative pathways for relaxation. Hence this spatial separation leads to high optical efficiency.

The mechanism for the carrier localization is a quantum effect related to the structure geometry: the ground state energy of a GaAs/InGaAs/GaAs quantum well is lower than that of a vacuum/InGaAs/GaAs quantum well. In the plane perpendicular to the wire direction Schrödinger's equation does not separate into two one-dimensional problems. We solve Schrödinger's equation (with standard boundary conditions) using an efficient, yet simple, finite-element approach. Results for the ground electronic wave function are shown in Fig. 1. Photoluminescence (PL) data for the electron-hole recombination are blue-shifted from the quantum well results, owing to the lateral localization. A plot of this shift is shown as a function of wire width in Fig. 2, where excellent agreement is seen between the experiment and our calculations. It is worth emphasizing that the calculation contains no fitable parameters. This agreement between experiment and theory tells us that these wires are of high quality and that their electronic properties can be understood quantitatively on the basis of the stuctures' measured geometry.

We have also studied the higher-lying states of the wires, of which theoretical considerations indicate that there should be several for these widths. Based on our interactions with the Forchel group we have motivated new experiments involving the use of excitation spectroscopy [10]. The experiments have measured blue-shifts for

the lowest three wire localized states (Fig. 3).

A related issue involves the effects of a magnetic field ($B \approx 9$ T) upon the spectra of the barrier modulated wires. The Forchel group has taken high excitation PL data for the $B-$field dependence of the lowest three wire localized states. These data exhibit an interesting transformation from wire-induced lateral localization at low fields to Landau localization at high fields. We have developed a theoretical approach to include the magnetic field and are currently preparing a manuscript which contains these results.

Another issue concerns the barrier modulated quantum *dots* fabricated by the Forchel group. A diagram of such a dot is shown as an inset to Fig. 1. As with the wires, these systems exhibit carrier states localized to the region under the barrier and the PL data is blue-shifted from the quantum well data. As for the wires, Schrödinger's equation for the dots does not separate into one-dimensional problems. We are in the process of using the finite-element approach to calculate the lowest few dot-localized states.

III. ELECTRON-PHONON INTERACTIONS IN NANOSTRUCTURES

During FY-93 we calculated electron-phonon scattering rates for quantum wires of GaAs embedded in AlAs [5]. As inputs to this calculation we needed the wave functions for the electrons, the "confined" phonons, and the "interface" phonons. For neither the electrons nor the phonons do the equations of motion separate into one-dimensional problems. Hence the solutions are nonanalytic. Even for the seemingly simple case of a wire having a square cross-section the electron and interface phonon wave functions cannot be calculated analytically. Recently we have developed efficient, yet simple, numerical techniques for calculating the electrons [4], the interface phonons [6], and the confined phonons [7] for *arbitrarily* shaped nanostructures (wires,

wells, dots, superlattices, etc.). This has enabled us to calculate the scattering rates for electrons in quantum wires having rectangular cross-sections.

For wire diameters ranging from 30 Å to 400 Å and electron energies ranging from 0 meV to 70 meV the scattering rate ranges from 4 $psec^{-1}$ to 200 $psec^{-1}$. For small (< 100 Å) wire diameters the interface phonons dominate the scattering rate and for large diameters the confined phonons dominate [Fig. 4(a)]. The intersubband scattering rate shows an interesting maximum when the intersubband energy splitting approximately equals the energy of an optical phonon [Fig. 4(b)]. We also tested the accuracy of various approximations for the electrons and phonons in wires. Separable approximations for the electronic wave functions give very accurate results, bulk GaAs approximations for the phonons give reasonable accuracy for large wire widths, and separable approximations for the interface phonons [8] give poor results, as does an approximation which incorporates only one confined phonon [8].

As part of this work we have also produced two general results, each of which serve to strengthen the fundamental soundness of certain semimacroscopic models of the electron-phonon interaction in nanostructures. In Ref. [9] we demonstrate that the effects of retardation are minimal in the calculation of the Fröhlich coupling for electron-phonon interactions. In Ref. [7] we demonstrate that the effect of mechanical boundary conditions on confined phonons can safely be ignored (Fig. 5).

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RELATED PUBLICATIONS

"Classical interface modes of quantum dots," P. A. Knipp and T. L. Reinecke, Phys. Rev. B **46**, 10310 (1992).

"Optical absorption due to interface phonons and interface plasmons of quantum dots," P. A. Knipp and T. L. Reinecke, Superlattices and Microstructures **12**, 553 (1992).

"Lateral quantization in the optical emission of barrier-modulated wires," Ch. Gréus, L. Butov, F. Daiminger, A. Forchel, P. A. Knipp, and T. L. Reinecke, Phys. Rev. B **47**, 7626 (1993).

"Barrier modulated semiconductor quantum wires," P. A. Knipp and T. L. Reinecke, J. Vac. Sci. Technol. B **11**, 1667 (1993).

"Electron-phonon scattering rates in quantum wires," P. A. Knipp and T. L. Reinecke, Phys. Rev. B **48**, 5700 (1993).

"Coupling of electrons to interface phonons in semiconductor quantum wells," P. A. Knipp and T. L. Reinecke, Phys. Rev. B (to appear in 15 October 1993 issue).

"The effects of boundary conditions on confined optical phonons in semiconductor nanostructures," P. A. Knipp and T. L. Reinecke, Phys. Rev. B (accepted).

"Electron-phonon scattering rates in quantum wires," P. A. Knipp and T. L. Reinecke, Solid-State Electron. (submitted).

"Photoluminescence excitation study of lateral subband structure in barrier modulated $In_{0.09}Ga_{0.91}As$ quantum wires," Ch. Gréus, R. Spiegel, F. Faller, A. Forchel, P. A. Knipp, and T. L. Reinecke, Phys. Rev. B (manuscript in preparation).

RELATED PRESENTATIONS

20th Annual Conference on the Physics and Chemistry of Semiconductor Interfaces, Williamsburg, VA, 25-29 January 1993:

"Barrier-modulated semiconductor quantum wires," P. A. Knipp and T. L. Reinecke.

March Meeting of the American Physical Society, Seattle, WA, 22-26 March 1993:

"Electron-phonon scattering rates in quantum wires," P. A. Knipp and T. L. Reinecke.

Annual Meeting of the Virginia Academy of Sciences, Norfolk, VA, 19-21 May 1993:

"Electron-phonon interactions in semiconductor quantum wires," P. A. Knipp and T. L. Reinecke.

6th International Conference on Modulated Semiconductor Structures, Garmisch, Germany, 23-27 August 1993:

"Electron-phonon scattering rates in quantum wires," P. A. Knipp and T. L. Reinecke.

RELATED RECOGNITION

1992 NRL Alan Berman Research Publications Award

FIGURES

FIG. 1. The calculated wave function for the ground electronic state of a barrier modulated wire of width 32 nm. The InGaAs quantum well lies between $0 < y < 5$ nm, the GaAs barrier lies between -16 nm $< x < 16$ nm, and the GaAs substrate lies in the region $y > 5$ nm. The wave function has no nodes and is symmetric around $x = 0$. Only the $x > 0$ half of the wave function is shown here. The inset shows the geometry of the barrier-modulated structures. If the diagram is translated into the page it represents a quantum wire, or if it is rotated about the $y-$axis it represents a quantum dot. Most of the carrier wavefunction is localized inside the dashed line.

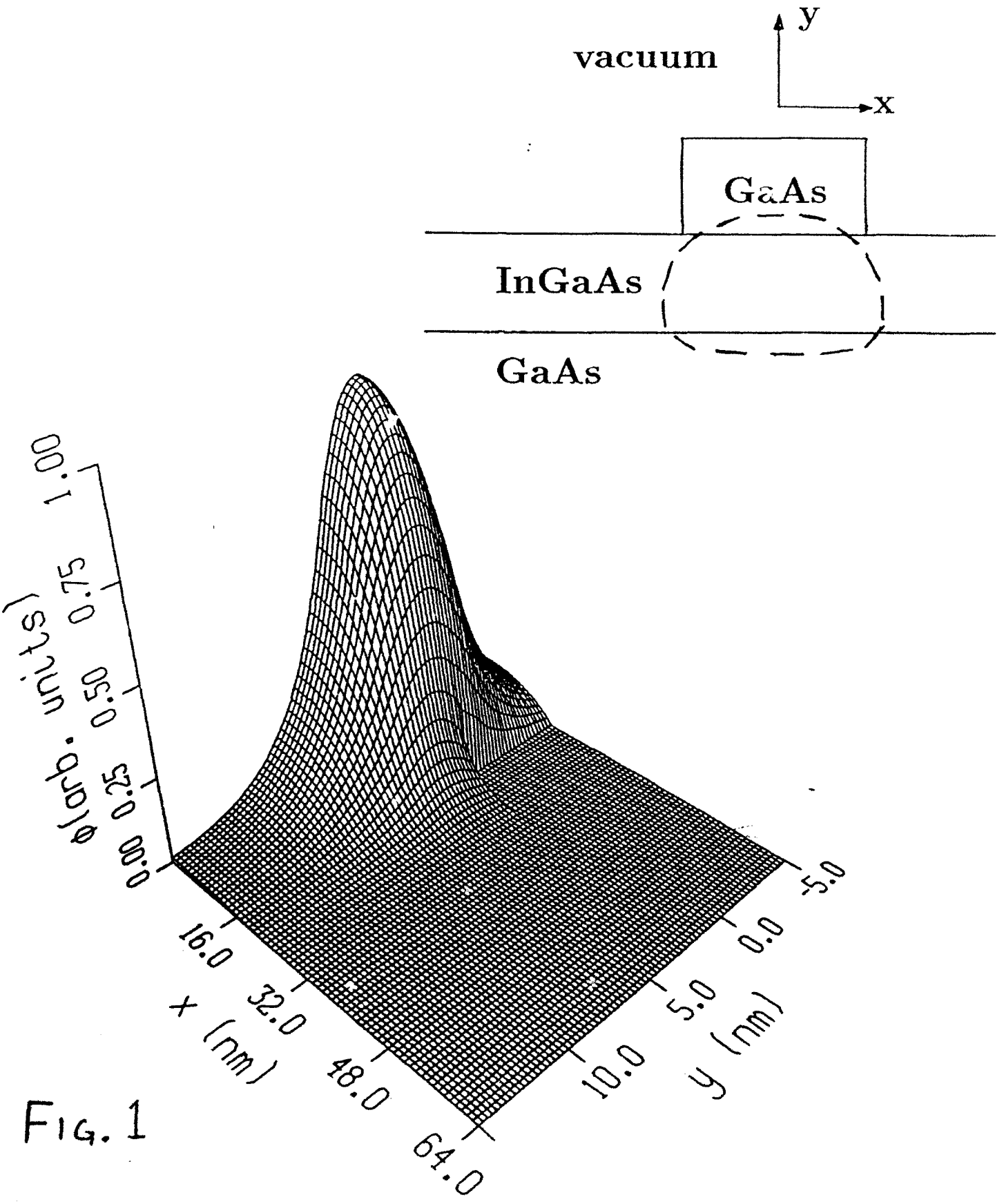
FIG. 2. The dependence of the quantum wire transition energy E on the wire width L. Circles and crosses correspond to different samples of Ref. [4]. The solid line gives the results of our calculation.

FIG. 3. Wire width dependence of the transition energies of the lowest three quantum wire subbands. The positions of the photoluminescence emission (PLE) peaks are marked by the crosses. The triangles, circles, and diamonds are the experimental PLE data for recombinations of the ground, first-excited, and second-excited wire states, respectively. The solid, dashed, and dotted lines are the results of our calculations corresponding to these transitions.

FIG. 4. (a) Intrasubband and (b) intersubband phonon emission rates as functions of the wire width r. The initial electron energy is chosen to be 60 meV above the bottom

of the initial electronic subband. The total rate is given by the solid line, and the rate from a model of bulk GaAs (AlAs) phonons is given by the dot-dashed (long dashed - short dashed) line. Contributions from the confined phonons, the AlAs-like interface phonons, and the GaAs-like interface phonons are respectively given by the dotted, the short-dashed, and the long-dashed lines.

FIG. 5. Comparison of the structure factors $\rho(z, z')$ which comprise the electron-phonon interaction in a quantum well of thickness $2a$ for confined optical phonons which (a) do not satisfy or (b) do satisfy mechanical boundary conditions at the interfaces. The dot-dashed, dashed, dotted, and solid lines indicate the incorporation of a number of phonons equalling 1, 3, 10, and ∞, respectively. Note that the converged results (i.e. solid lines) for (a) and (b) are identical.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y
x
GaAs
InGaAs
GaAs
log10 (arb. units)
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0.50
0.25
0.00
16.0
32.0
48.0
64.0
x (nm)
-5.0
0.0
5.0
10.0
y (nm)

FIG. 1

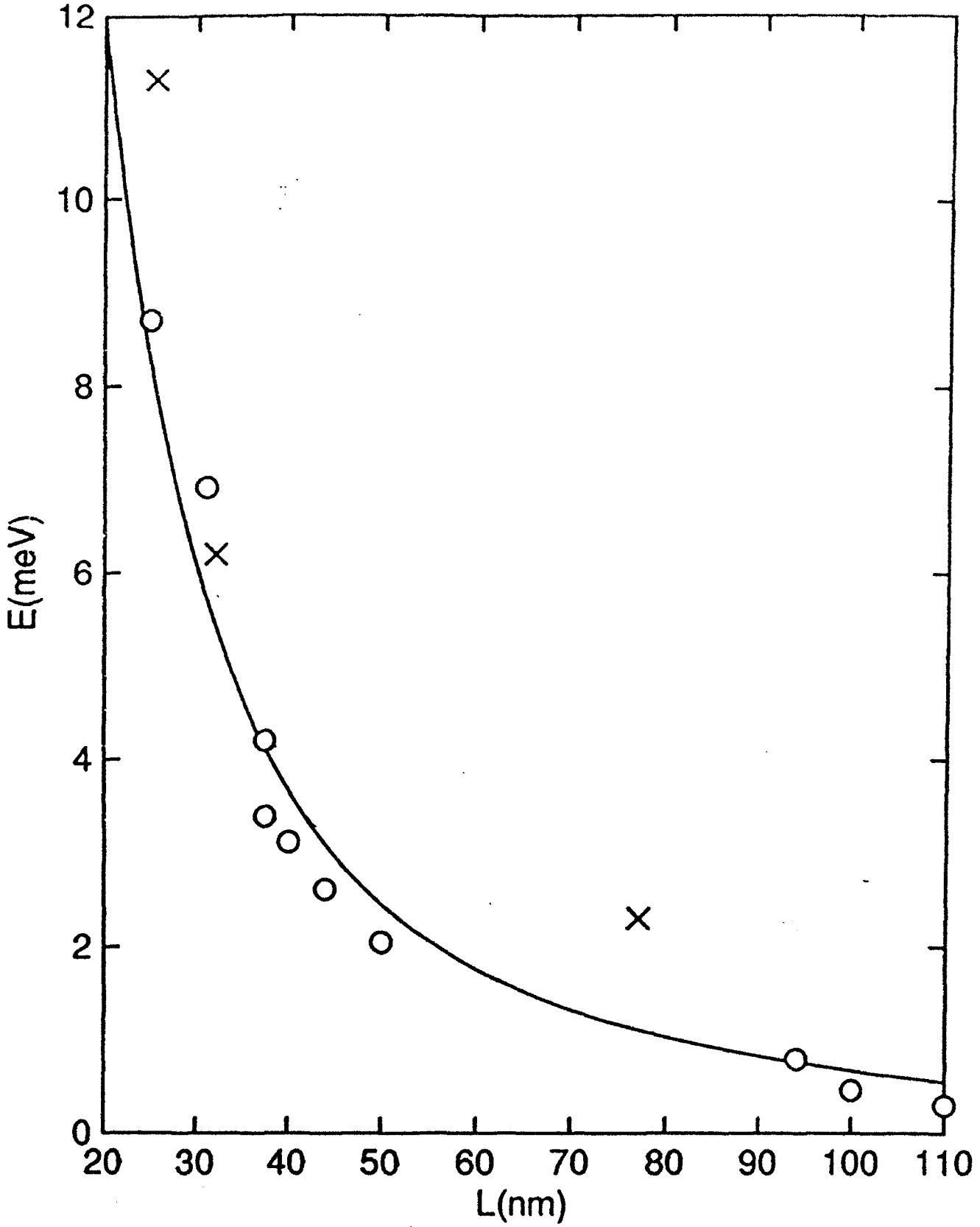

FIG. 2

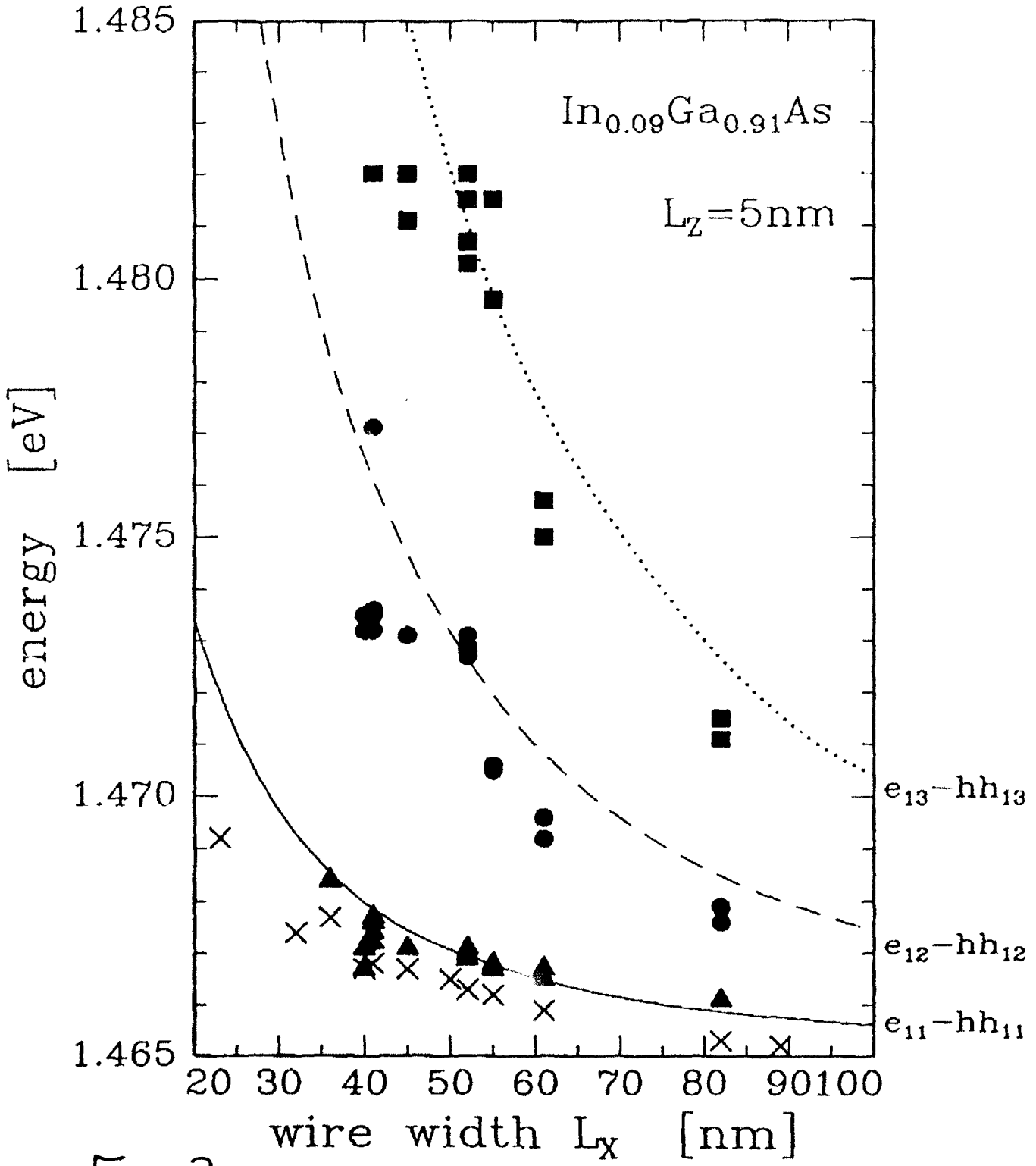
1.485
1.480
1.475
1.470
1.465
energy [eV]
$In_{0.09}Ga_{0.91}As$
L_Z=5nm
e_{13}–hh_{13}
e_{12}–hh_{12}
e_{11}–hh_{11}
20 30 40 50 60 70 80 90100
wire width L_X [nm]

FIG. 3

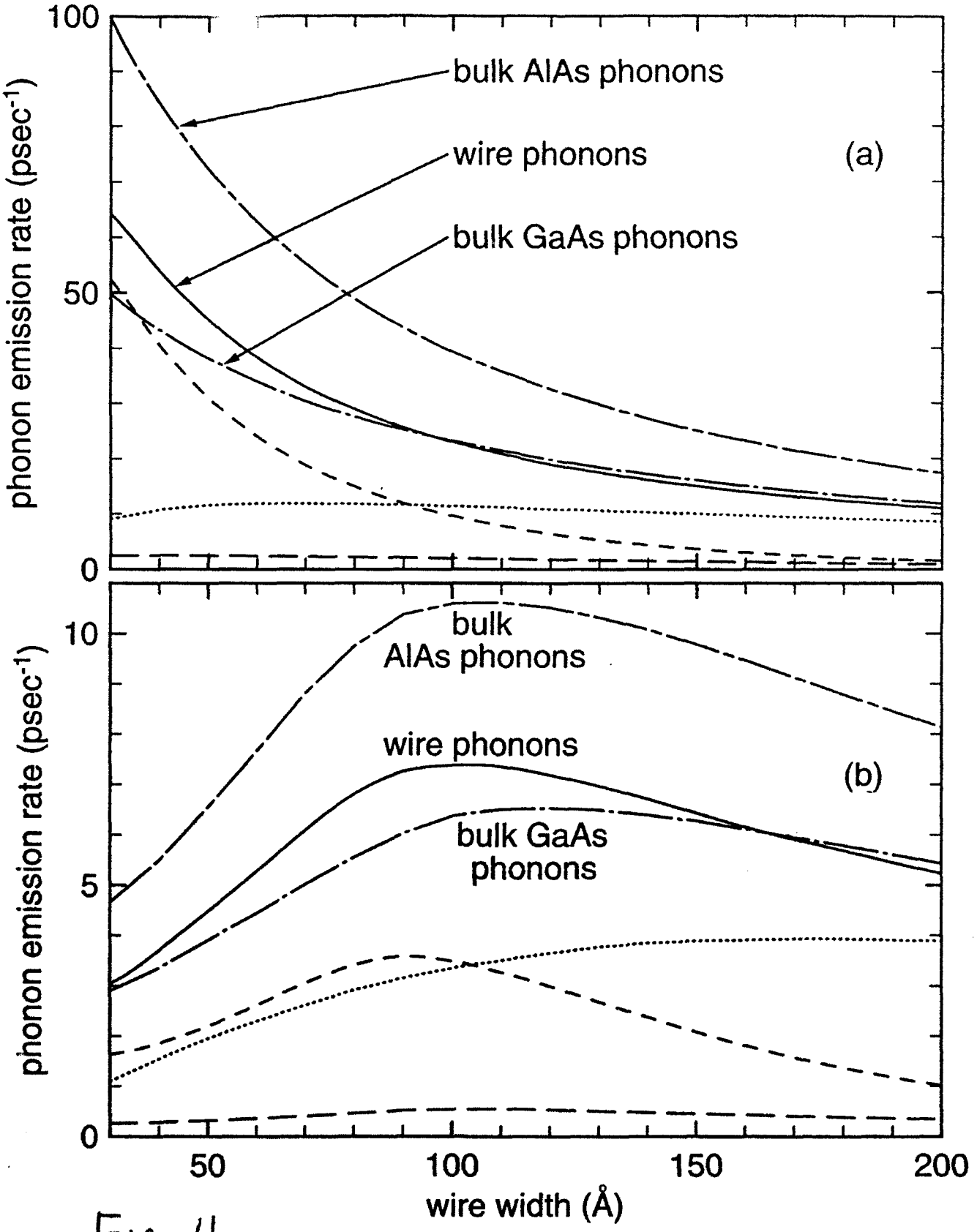
100
50
0
phonon emission rate (psec^{-1})
bulk AlAs phonons
wire phonons
bulk GaAs phonons
(a)
10
5
0
phonon emission rate (psec^{-1})
bulk
AlAs phonons
wire phonons
bulk GaAs
phonons
(b)
50
100
150
200
wire width (Å)

FIG. 4

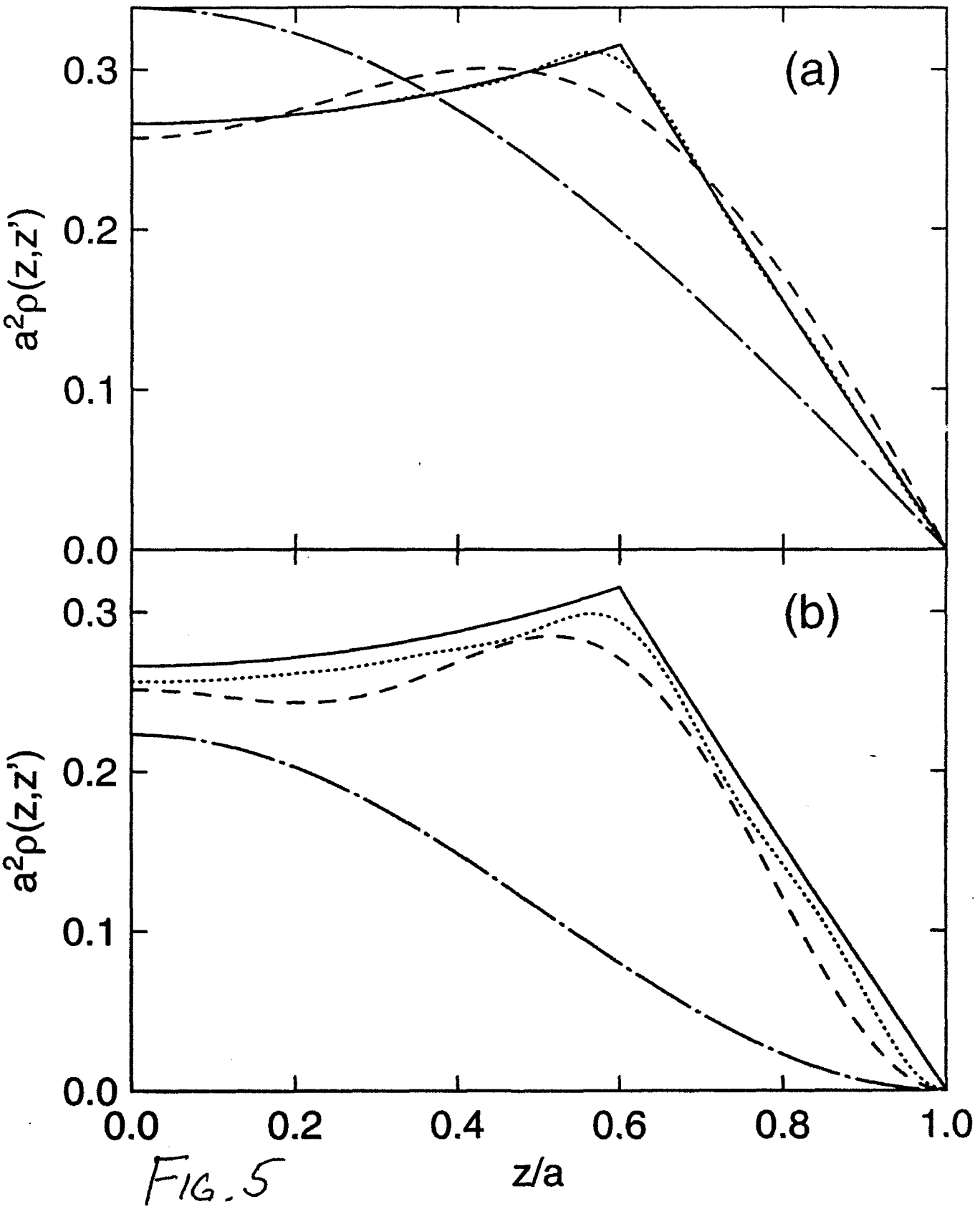

FIG. 5