

# 以數值方法計算矽銻半導體之?量子井結構

劉昌杰、韓斌

E-mail: 9125198@mail.dyu.edu.tw

## 摘要

本論文所討論的是以數值方法計算矽銻半導體之?量子井結構，利用量子力學中有限深能井的模型，說明半導體兩種晶格常數不相同的材料，此種異質界面要成長成為晶格匹配的材料時所承受的應變知識和量子井的構造，進而再利用薛丁格方程式 (SCHRODINGER EQUATION) 和MODEL-SOLID THEORY的理論探討計算量子井中，因摻雜濃度X值時的價電帶和導電帶可能侷限的能階大小，再考慮激子的束縛能，得到量子井可能的發光能量。從理論的計算結果我們可由電磁波光譜表上查得所要的光波頻率。由研究計算分析結果中得摻雜濃度和井厚度的比例控制，均將影響到半導體的光學特性。

關鍵詞：無

## 目錄

第一章 緒論--P1 第二章 理論背景 2.1 GEXSI1-X 的基本性質--P4 2.2應變產生的原因--P7 2.3應變對能帶結構的影響--P8 2.4單子井結構與能帶--P9 2.5量子井束縛能階的計算--P10 2.5.1 MODEL-SOLID THEORY--P10 2.5.2 SCHRODINGER EQUATION--P13 2.6光與能階躍遷--P18 2.7半導體材料與波長之關係--P19 第三章 GEXSI1-X / SI半導體?量子井之研究分析 3.1 GEXSI1-X 摻雜各參數的獲得--P21 3.2 GEXSI1-X 摻雜能階及量子井之計算--P23 3.3計算結果討論--P26 第四章 結論--P30 參考文獻--P47

## 參考文獻

- 1.L.ESAKI AND R.TSU,"SUPERIATTICE AND NEGATIVE DIFFERENTIAL CONDUCTIVITY IN SEMICONDUCTER -S", IBM J.RES.DEVELOP.VOL.14,PP.61-63 (1970).
- 2.G.W.WICKS,"MOLECULAR BEAM EPITAXY OF - SEMICONDUCTORS",CRITICAL REVIEWS IN SOLID STATE AND MATERIALS SCIENCES VOL.18,PP.239-243 (1993).
- 3.A.Y.CHO,"GROWTH OF PERIODIC STRUCTURES BY THE MOLECULAR-BEAM METHOD",APPL.PHYS.LETT.VOL .19,PP.467-470 (1971).
- 4.Y.KAWAI AND T.YAMADA,"LOW TEMPERATURE-STRESSED AGING TEST OF 1.3-1.45  $\mu$  M LASER DIODES UNDER HIGH POWER OPERATION",ELECTRONICS LETTERS,VOL.26,PP.53-55 (1990).
- 5.A.PERALES,L.GOLDSTEIN,B.FERNIER,C.STARCK,J.L.LIEVIN,F.PEINGT,AND J.BENOIT,"MULTI-QUANTUM WELL LASERS EMITTING AT 1.5  $\mu$  M GROWN BY GSMBE",ELECTRONICS LETTERS,VOL.25,PP.1350- 1352(1990).
- 6.G.C.OSBOURN,J.APPL.PHYS.53,1586 (1982).
- 7.C.G.VAN DE WALLE AND R.M.MARTIN,PHYS.REV.B 35.8154 (1987).
- 8.C.G.VAN DE WALLE AND R.M.MARTIN,PHYS.REV.B 34. 5621 (1986).
- 9.J.BARDEEN AND W.SHOCKLEY,PHYS.REV.80,72 (1950).
- 10.R.M.MARTIN AND C.G.VAN DE WALLE,BULL.AM.PHYS.SOC.30 (3). 226 (1987).
- 11.C.G.VAN DE WALLE AND R. M. MARTIN (UNPUBLISHED).
- 12.C.G.VAN DE WALLE,PH.D.DISSERTATION,STANFORD UNIVERSITY,1986.
- 13.C.G.VAN DE WALLE AND R.M.MARTIN,J.VAC.SCI. TECHNOL.B4,1055(1986)
- 14.L.C.FELDMAN,J.BEVK,B.A.DAVIDSON,H.J.GOSSMAN,AND J.P.MANNAERTS,PHYS.REV.LETT.59,664(1987)
- 15.L.KLEINMAN,PHYS.REV.128, 2614 (1962).
- 16.H.J.MCSKIMIN,J.APPL.PHYS.24,988(1953); H.J.MCSKIMIN AND P.ANDREATCH JR.,IBID.35,3312(1954).
- 17.C.W.GARLAND AND K.C.PARK,J.APPL.PHYS. 33, 759 (1962).
- 18.J.D.WILEY,IN SEMICONDUCTORS AND SEMIMETALS,EDITED BY R.K.WILLARDSON AND A.C. BEER(ACADEMIC,NEW YORK,1975),VOL.10.
- 19.D.GERLICH,J.APPL.PHYS.34.813 (1963).
- 20.W.F.BOYLE AND R.J.SLADEK,PHYS.REV.B 11, 2933 (1975).
- 21.F.S.HICKERNELL AND W.R.GAYTON,J.APPL.PHYS.37,462 (1966).
- 22.W.F.BOYLE AND R.J.SLADEK,PHYS.REV.B 11,1587 (1975).
- 23.D.I.BOLEF AND M.MENES,J.APPL.PHYS.31,1426 (1960).
- 24.I.O.BASHKIN AND G.I. PERESEDA,FIZ. TVERD. TELA(LENINGRAD)16,3166 (1974)[SOV.PHYS.SOLID STATE 16, 2058 (1975)].
- 25.D.BERLINCOURT,H.JAFFE,AND L.R.SHIOZAWA, PHYS. REV. 129. 1009(1963).
- 26.R.B.HALL AND J.D.MEAKIN,THIN SOLID FILMS 63, 203 (1979).
- 27.R.D.GREENOUGH AND S.B.PALMER,J.PHYS.D 6, 587 (1973).
- 28.R.I.COTTAM AND G.I.SAUNDERS,J.PHYS.CHEM.SOLIDS 36, 187(1975).
- 29.LANDOLT-BORNSTEIN, NUMERICAL DATA AND FUNCTIONAL RELATIONSHIPS IN SCIENCE AND TECHNOLOGY (SPRINGER, NEW YORK,1982),GROUP 1, VOL.17A-B.
- 30.W.A.HARRISON,E.A.KRAUT,J. R.WALDROP,AND R.W.GRANT,PHYS.REV.B18.4402(1978);R.M.MARTIN,J. VAC.SCI. TECHNOL.17,978(1980).
- 31.K.KUNC AND R.M.MARTIN,PHYS.REV.B24,3445(1981).
- 32.P.HOHENBERG AND

W.KOHN,PHYS.REV.136,B864(1964);W.KOHN AND L.J.SHAM,IBID.140,A1133(1965) ;EXCHANGE AND CORRELATION POTENTIALS ARE BASED ON THE DATA FROM D.M.CEPPERLEY AND B.J.AL -DER,PHYS.REV.LETT.45,566(1980),AS PARAMETRIZED BY J. PERDEW AND A. ZUNGER,PHYS.REV.B23 ,5048(1981). 33.SEE, E.G.,O.H.NIELSEN AND R.M.MARTIN,PHYS.REV.B32,3792(1985). 34.G.B.BACHELET,D.R.HAMANN,AND M.SCHLUTER,PHYS.REV.B 26,4199(1982). 35.RECENT QUASIPARTICLE-ENERGY CALCULATIONS CONFIRM THIS ASSESSMENT;SEC M.S.HYBERTSEN AND S.G. LOUIE, PHYS. REV. B 34, 5390(1986). 36.L.KLEINMAN, PHYS. REV. B 24, 7412 (1981). 37.ATOMIC CONFIGURATIONS ARE LISTED IN REF.2,AND WERE OBTAINED FROM TIGHT-BINDING CALCULAT -IONS BY D.J.CHADI(PRIVATE COMMUNICATION).THE SENSITIVITY OF THE MODEL-SOLID VALUES TO THE CHOICE OF CONFIGURATION WAS DISCUSSED IN REF. 2 38.C.G.VAN DE WALLE AND R. M. MARTIN, PHYS. REV. B 37 4801 (1988). 39.F.H.POLLAK AND M. CARDONA,PHYS .REV. 172, 816 (1968). 40.D.W.LANGER, R. N. EUWEMA, K. ERA, AND T. KODA, PHYS. REV. B 2, 4005 (1970). 41.W.C.HERRING AND E. VOGT, PHYS. REV. 101, 944 (1956); L. BALSLEV, IBID. 143, 636 (1966). 42.E.O.KANE PHYS. REV. 178, 1368 (1969). 43.J.WILSON/ J.F.B. HAWKES, OPTOELECTRONICS AN INTRODUCTION 2ND ED., PRENTICE HALL 1989 BEN G.STREETMAN,SOLID STATE ELECTRONIC DIVICES 2ND ED.,PRENTICE HALL 1980