文章编号:1004-5929(2004)01-0044-04

p 型掺杂 Si/Ge 量子点的电子拉曼散射

谭平恒[1,2],周 霞[1],杨富华[1],BOUGEARD D[2],SABATHIL H[2],VOGL P[2],
ABSTREITER G[2],BRUNNER K[2]
(1. 半导体超晶格国家重点实验室,中科院半导体研究所,北京 100083;
2. Walter Schottky Institut, Technische Universität München, D-85748 Garching, Germany)

摘 要: 在本文中我们首次报道了p型掺杂的自组织Si/Ge量子点中空穴能级子带间的电子拉曼散射,此电子跃迁的能量为105 meV。Si/Ge量子点Ge-Ge模的共振拉曼散射表明此空穴能级间的电子拉曼散射与Γ点附近的E_0($\approx$2.52 eV)发生了共振,而E_1的能量小于2.3 eV. 变温实验和偏振实验进一步证实了我们的指认。所有观测的实验数据与6-band k·p能带结构理论的计算结果吻合得很好。

关键词: 量子点;电子拉曼散射;共振拉曼散射
中图法分类号:O657.37 **文献标识码**:A

Electronic Raman Scattering in p-doped Self-Assembled Si/Ge Quantum Dots

TAN Ping-heng[1,2], ZHOU Xia[1], YANG Fu-hua[1], BOUGEARD D[2], SABATHIL H[2], VOGL P[2], ABSTREITER G[2], BRUNNER K[2]
(1. *State Key Laboratory for Superlattices and Microstructures*, *P. O. Box* 912, *Beijing* 100083, *P. R. China*; 2. *Walter Schottky Institut*, *Technische Universität München*, *D*-85748 *Garching*, *Germany*)

Abstract: The first resonant electronic Raman spectroscopy study of discrete electronic transitions within self-assembled Si/Ge quantum dots (QD) is reported in this paper. A Raman transition of localized holes with a dispersionless energy of 105 meV and a resonance energy to virtually localized electrons at the direct band gap $E_0\approx$2.52 eV far above the indirect fundamental band gap of Si/Ge are observed. Both values are in agreement with 6-band k·p band structure calculations for such QDs.

Key words: quantum dots; electronic Raman scattering

Raman scattering has long been known as a powerful tool for characterization of electronic as well as the structural and vibrational properties of bulk semiconductors and also nanostructural and heterostructured semiconductors.[1,2] Owing to the tunability of the incident photon energy, the resonant electronic Raman measurement provides additional information, that is, selectivity in the momentum space in exploiting the electronic band structures.[3] In this paper, we report the first study on the resonant electronic Raman spectroscopy of discrete electronic transitions within p-doped self-assembled Si/Ge quantum dots (QD), from which some key parameters of the band structure of Si/Ge quantum dots are deter-

收稿日期:2003-07-22

mined experimentally.

The Si/Ge QD samples were grown by a solid-source molecular beam epitaxy on n − (100) Si substrates in the Stranski-Krastanow growth mode at a substrate temperature of 510℃.[4] Each sample contains 80 Si/Ge QD layers separated by 25 nm Si with a boron modulation doping in the centre and is capped with 100 nm Si. Several samples have been annealed at temperatures from 600℃ to 800℃ for one hour. Micro-Raman measurements were performed at 6 K in backscattering geometry with a spectral resolution of 3.8 cm^{-1} using a triple Raman spectrometer equipped with a liquid nitrogen cooled Si charge coupled device camera system. The samples have been studied at Raman excitation energies ranging from 1.83 eV (677 nm) to 3 eV (413 nm) using Argon ion and Krypton laser lines. The laser was focused to a spot of about 1 μm with a laser power of 0.3 mW on the sample.

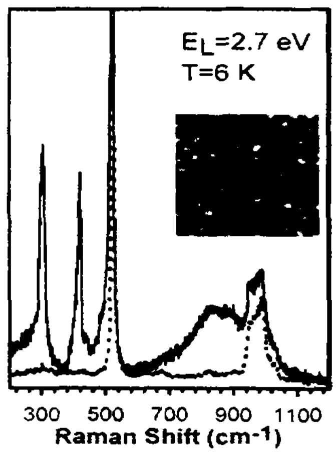

Fig. 1 Raman spectra of a Si/Ge QD sample (solid line) and a Si substrate (dotted line). The inset shows an AFM image (200 × 200 nm) of an uncapped Si/Ge QD sample.

The inset of Fig. 1 shows an AFM image of the uncapped reference sample. The Si/Ge QDs are elongated hut clusters. The lateral size is about 15×25 nm^2, the height about 2 nm and the sheet density 1.5×10^{11} cm^{-2}. A detailed and quantitative phonon Raman scattering characterization of these structures has been performed earlier.[2] It revealed structural parameters affecting the QD band structure, such as Ge content and strain. The phonon Raman study showed that the interface region between Ge rich regions within small as-grown Si/Ge QDs and their Si environment is very sharp.

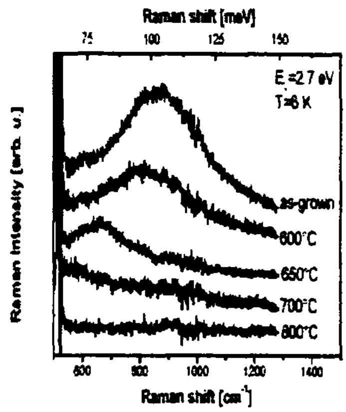

Fig. 2 Raman spectra of a Si/Ge sample annealed at different temperatures.

Fig. 1 shows the Raman spectra of as grown Si/Ge QD sample and a Si substrate excited by a 457 nm laser. Because of the weak resonant effect of most 2nd acoustic Raman modes, the Raman signal from Si/Ge QDs can be clearly distinguished from that of Si substrate and spacer layers. Besides the Raman peak of Ge-Ge and Si-Ge peaks of Si/Ge dots, there is an additional peak at 850cm^{-1}(105meV) with a FWHM of 25 meV. This band is found to be no dispersion with varying the laser excitation energy, and thus, can be attributed to a dispersionless intraband transition of localized holes in Si/Ge dots.

Fig. 2 shows the Raman spectra of Si/Ge dot samples annealed at different temperatures, in which all Raman spectra are subtracted from the Raman signal of a pure Si substrate. Annealing the Si/Ge dots for an hour from 600 ℃ to 800 ℃ results in a significant red shift of the 850cm^{-1}-peak with increasing the annealing temperature. For the Raman spectrum of Si/Ge dots annealed at 800 ℃, the redshifted peak can not be distinguished from the phonon modes of Si/Ge dots below 500 cm^{-1}. The redshift of the 850cm^{-1}-peak and its broad spectral feature further confirms its dot nature, rather than a disorder or dislocation induced Raman modes. The intermixing of Si-Ge increases with the annealing temperature. The Ge content will be reduced in the annealing process, but almost keeps constant within the island core. This result is explained by a large Si diffusion constant within Ge-rich regions in Si/Ge dots and has been shown by phonon Raman scattering.[2] With increasing intermixing, Ge-content, Strain and the strain-induced splitting between hh and lh states decrease. The quantum confinement along the growth direction is also reduced. Therefore, the redshift of the $850cm^{-1}$-peak is a result of the modification of the band structure of Si/Ge dots with the increasing annealing temperature.

The Raman spectra of as-grown Si/Ge dots are measured under variation of the excitation energy from 1.83 eV to 3 eV. Fig. 3 shows the integrated intensities of the Ge-Ge phonon mode and the hh-lh transition depending on the Raman excitation energy. Both peaks are contributed from the Si/Ge dots whereas Ge wetting layers contributions to the remnant Raman spectrum can be neglected. The Ge-Ge phonon mode shows two resonant peaks at about 2.3 eV and 2.52 eV. The resonance at 2.3 eV is close to the E_1 and $E_1 + \Delta_1$ gap in bulk Ge,[5] this resonance at momentum vectors along the {111}-directions of the Brillouin zone is not observed for the hole transition. A common resonance of the phonon mode and the electronic intra valence band transition is observed around 2.52 eV. This Raman resonance is assigned to the direct band gap E_0 of localized hh and virtually bound Γ-electron states within the small-sized Si/Ge dots.

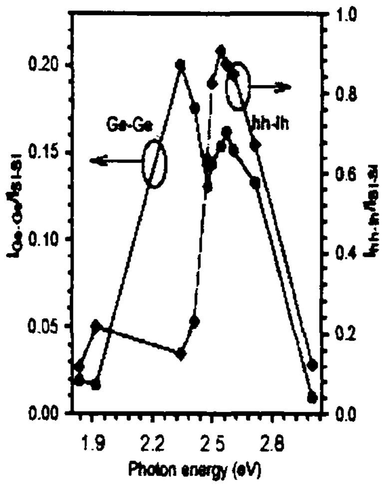

Fig. 3 Integrated intensity of Ge-Ge phonon and hh-lh transition vs. laser energy.

The QD structures have also been characterized by phonon Raman scattering and XRD. An average Ge content of 80% and lateral strain of -3.4% close to the biaxial case has been determined for the core of as-grown QDs.[2] AFM studies of uncapped Ge QDs reveal a lateral size of 20 nm and a height of about 2 nm. These structural parameters served as an input for valence band structure model calculations using the 6-band k·p simulator $nextnano^3$ including elastic strain relaxation in lens-shaped QDs. The calculations yield a splitting energy between hh- and lh-like ground states of 101 meV and a direct E_0 gap of 2.3 eV which agree well with the observed Raman results. These non-refined simulations also predict a type-II fundamental band gap of 770 meV and a lateral quantum confinement energy for holes of 42 meV that are close to previous PL and admittance results.[6,7]

In conclusion, we have presented the first resonant electronic Raman spectroscopy study of discrete electronic transitions in small *p*-doped Si/Ge QDs. An intraband transition of localized holes with energy of 105 meV is observed as a broadened Raman line. It is attributed to a hh-lh-transition within the QDs. Due to significant intermixing of Si and Ge, i.e. reduced strain-induced hh-lh splitting and quantum confinement, this transition energy shifts to lower values with increasing annealing temperature. The hh-lh transition Raman efficiency shows a clear resonance at excitation energy of 2.5 eV. This resonance energy is attributed to the direct band gap E_0 between localized states in the Si/Ge QDs.

参考文献:

[1] Kanehisa M A, Wallis R F, Balkanski M, Interband electronic Raman scattering in p-silicon[J]. Phys. Rev. B, 1982, 25: 7619.

[2] Tan PH, Brunner K, Bougeard D, Abstreiter G, Raman characterization of strain and composition in small-sized self-assembled Si/Ge dots[J]. Phys. Rev. B, 2003,12:125302.

[3] Kwok SH, Yu PY, Tung CH et al., Confinement and electron-phonon interactions of the E1 ex-

citon in self-organized Ge quantum dots[J]. Phys. Rev. B, 1999, 59:4980.
[4] Brunner K, SiGe nanostructures[J]. Rep. Prog. Phys., 2002, 65:27.
[5] Schorer R, Abstreiter G, Kibbel H et al., Resonant-Raman-scattering study on short-period Si/Ge superlattices[J]. Phys. Rev. B, 1994, 50: 18211.
[6] Zhang SK, Zhu HJ, Lu F et al., Coulomb Charging Effect in Self-Assembled Ge Quantum Dots Studied by Admittance Spectroscopy[J]. Phys. Rev. Lett., 1998, 80: 3340.
[7] Asperger TH, Miesner CH, Brunner K, Abstreiter G, Space Charge Spectroscopy of Self Assembled Ge Quantum Dots in Si[J]. Phys. Stat. Sol. (b), 2001, 224:237.