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Photoluminescence of 8H-SiC

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Abstract. 8H-SiC epilayers grown on small 8H-SiC Lely platelets are investigated optically using photoluminescence spectroscopy. At low temperature the near band gap emission detected in the 2.78 to 2.67 eV range contains sharp lines associated to nitrogen-bound-exciton recombination. Three different no-phonon lines are detected accompanied by their phonon replicas. Free-exciton replicas are also observed which allows the determination of the excitonic band gap. The binding energy of the bound excitons can thus be determined and the ionization energies of the three nitrogen levels in 8H-SiC are estimated and found to be rather shallow compared to the values for other hexagonal polytypes. Additional bound-exciton lines are observed when the experimental photoluminescence temperature is increased.

Introduction

Degradation problems of bipolar devices have led to many studies of 8H-like stacking faults in 4H-SiC including high resolution transmission microscopy and photoluminescence (PL) [1,2]. In these studies the 8H polytype material appears as very small inclusions of few nm size. The PL appears even at low temperature as broad features in the range 460 - 475 nm (about 2.70 to 2.61 eV) which represent the phonon replicas of a material with excitonic bandgap (E_{gx}) at about 2.71 eV. Considering the hexagonality [3] the excitonic bandgap of 8H polytype was evaluated to be E_{gx} = 2.80 ± 0.015 eV. The indirect bandgap was reported in the literature to be 2.86 eV [4,5], however the experimental data are unclear. Here PL results on epitaxial layers of the 8H SiC polytype are presented and analyzed to allow determination of E_{gx} as well as the binding energy of the nitrogen bound excitons.

Experimental procedure

8H-SiC Lely platelets were used as substrates. Beside the experimental work described here, micro-Raman spectroscopy and thermal oxidation were used to determine the polytype and the polarity of the substrates [6]. The substrates were polished to obtain an off angle of ~ 5^o toward the [11-20] direction. The epilayers were grown by chemical vapor deposition with silane and propane as precursors. They were intentionally doped which resulted in a nitrogen concentration of 10^{16} cm^{-3} and their thickness was about 10 µm. The samples were cut into two parts: one was used for structural investigations, whereas the other for optical studies.

Transmission electron microscopy (TEM) investigations were done, using a microscope operated at 300 kV. The images were taken from cross-section of the samples which were prepared as lamella using a standard focus ion beam procedure to get electron transparency.

For the photoluminescence the sample was excited by either the 244 nm line of a FreD (Ar+) laser or the 351 nm of an Ar^+ ion laser. The PL spectra were recorded by using a single monochromator and a UV sensitive CCD camera. The resolution for the system is about 0.26 meV for this study. The sample was either placed in a bath cryostat to record the PL spectra at 1.8 K or in a temperature variable cryostat with the possibility to obtain temperature between 5 K and room temperature. The spectra were recorded in the near back-scattering geometry which is a common geometry and allows recording mainly the luminescence with polarization perpendicular to the c-axis. The PL spectra were not corrected for the response of the monochromator and CCD.

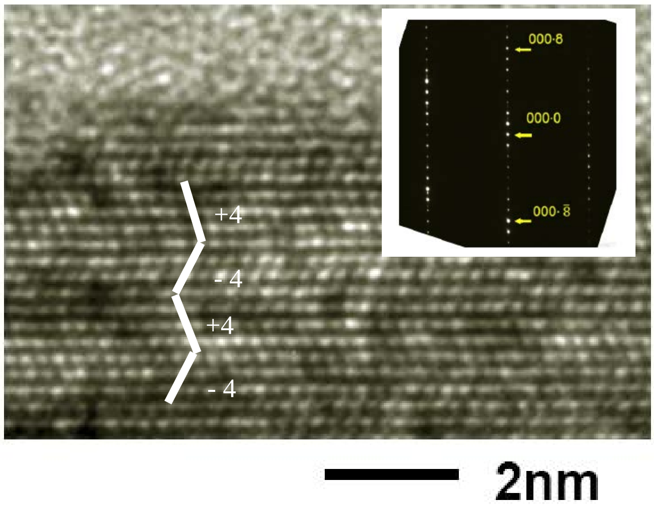

Fig.1: High resolution transmission electron microscopy image of the substrate showing the 8H structure. The inset shows the SAD pattern

Results.

High resolution transmission electron microscopy observed from the <11-20> direction revealed the <+4,-4> zigzag structure of the material as illustrated in Fig.1. The corresponding selected area diffraction (SAD) pattern with light and dark spots observed along the <0001> axis indicates a periodicity in the unit cell corresponding to the 8H polytype.

Typical PL spectra recorded at low temperature are presented in Fig.2. Sharp lines are observed in the range from 2.78 to 2.67 eV and they are dominating the PL spectra. They are associated to the near-band gap (NBG) emission which will be discussed more in detail in this paper. However when using the 351 nm line as excitation a broad band is also observed at lower energy (2.6 to 2.45 eV) with a typical shape associated to donor-acceptor pair (DAP, involving probably nitrogen donor and aluminiun acceptor) recombination in SiC; this luminescence is not observed when using the 244 nm line as excitation which has a smaller penetration depth than the 351 nm line. This DAP luminescence is suggested to be a contribution from the substrate.

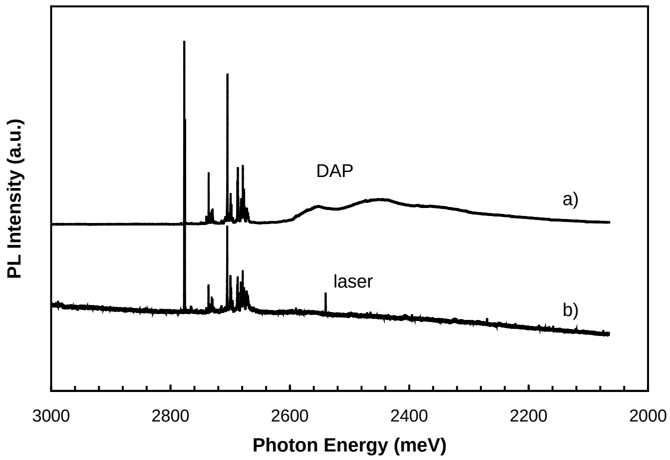

Fig. 2: PL spectra of the 8H-SiC layer recoded at a) 5K and b) 1.8 K and using as excitation line the a) 351 and the b) 244 nm line, respectively. The line labeled “laser” is located at 488 nm and is thus due to the second order of the laser line.

The NBG emission is shown in detail in Fig.3 and contains of many sharp lines which are related to the recombination of excitons bound to nitrogen donors as well as the recombination of free excitons (FE). In SiC, FE is only observed as recombination involving various conserving phonon replicas. However for shallow bound excitons (BE) the no-phonon (NP) line may be observed followed by its phonon replicas. The intensity of this NP line is expected to increase with the binding energy of the exciton and the corresponding nitrogen level. The number of phonon replicas is also depending on the polytype, four are recognized for the cubic polytype such as TA, LA, TO and LO. However the number of replicas is larger for the 4H and 6H polytype with 24 and 36 phonon replicas, respectively. In addition, not all phonon replicas are observed with the common experimental geometry, because of the polarization selection rules present in uniaxial crystals; i.e., some phonon replicas are polarized perpendicular to the c-axis, and some parallel to it (for general information

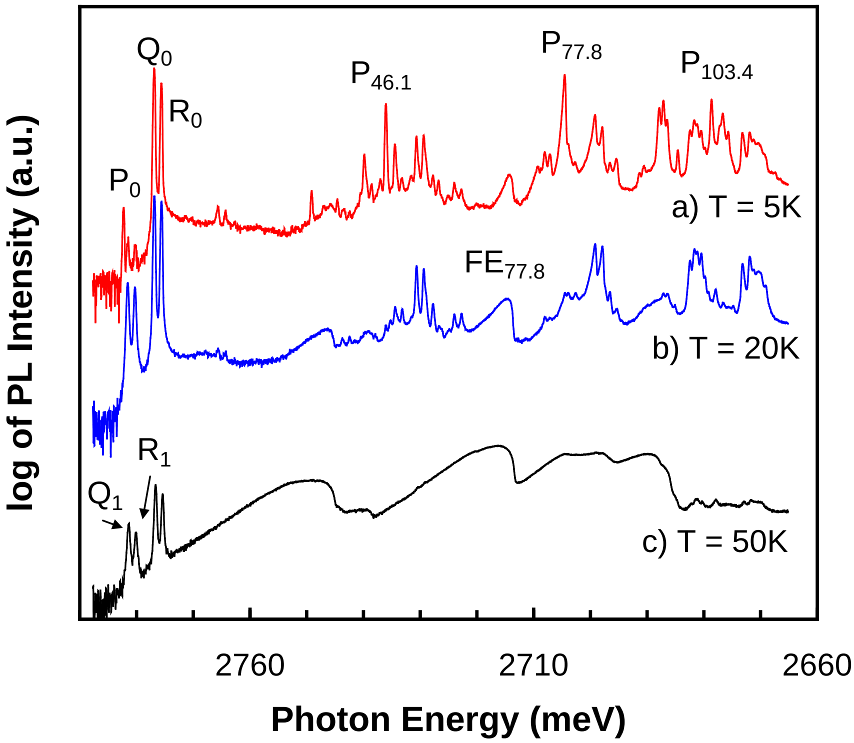

Fig.3 : PL spectra of the near band gap emission of the 8H-SiC layer recorded at various temperatures (note that the PL intensity scale is logarithmic to favor the visualization of weak

Table I: Phonons replicas observed in N doped SiC epilayers for polarization ⊥c . ** correspond to the observed lines for 8H.

	6H	4H	3C	8H	**
TA	36.2	33.2		33.1	P,Q,R
	40.3	41.1		42.1	P,Q
	46.3	46.3	46.3	46.3	P;Q,R
				47.8	P;Q
LA	53.5	50.9			
	67	68.1		68.9	P,Q,R,
				73.1	P
	77	76.3	79.3	77.8	P,Q,R
TO	94.7	94.5	94.3	94.5	P,Q,R
				95.2	P,Q
	95.6	96		95.8	P,
		98.9		97.5	P
LO	104.2	103.9	102.3	103.5	P,Q,R
				105.6	P
	107	106.8		106.6	P,Q,R

regarding PL in SiC see the review of Janzén et al [7]). In 8H polytype 48 phonon replicas are expected and probably 24 of them should be polarized perpendicular to the c-axis. Table I summarizes the various phonon energies observed for this 8H polytype compared with other polytypes.

The observed three lines at high energy in the spectrum of Fig.3.a and labeled as P_0, Q_0 and R_0 are associated to the no-phonon (NP) lines of the nitrogen bound exciton (N-BE); they are at 2782.4, 2777.1 and 2775.8 meV, respectively. In 8H SiC the number of inequivalent carbon sites should be four (4) and as nitrogen is replacing carbon in the SiC matrix we should expect four nitrogen levels in the band gap thus four NP N-BE lines. However, only three NP lines are observed here. Similar behavior has been reported for the rhombohedral polytypes 15R, 21R and 33R polytype where five, seven and 11 inequivalent sites exist but only four, six and ten NP N-BE lines are observed, respectively. Their phonon replicas are observed at lower energies with energy separations from the no-phonon lines very close to the phonon energies observed in other polytypes (as indicated by the number in subscript in Fig.3.a). In addition the free-exciton (FE) phonon replicas are also observed weakly due to the low temperature of the PL measurement and to the fact that the layer was slightly doped in the low 10^{16} cm^{-3} range, in analogy to the 4H or 6H polytype. From the energy shift of the FE phonon replicas with respect to the N-BE phonon replicas the excitonic band gap can be calculated assuming that phonons with the same energies are involved in the corresponding replicas for FE and N-BE. This excitonic band gap is found to be 2.79 eV, which is rather close to the value obtained by considering the hexagonality [3]. The binding energy of the N-BE can also be evaluated. If the Haynes rule is applied as described in Ref [8] the ionization energy for three of the nitrogen donors in 8H will be about 53, 74 and 79 meV, respectively. These values are rather shallow compared to those in the other hexagonal polytypes. The shallower is usually close to the value which could be predicted by the effective mass theory, however not enough parameters are known for the 8H polytype to complete the calculation.

When the temperature increased the N-BE P_0 line and its phonon replicas are rapidly quenched and are not observed above 15K (Fig.3.b). The N-BE Q and R are observed up to almost 60K. The energies obtained from the Arrhenius plot (intensity as function of the reciprocal temperature) are found to be very close to the binding energies of the three NP lines. In addition the broad FE related lines are easily recognized. Additional BE lines are observed (Q_1 and R_1 in Fig.3.c) which are interpreted as the excitonic recombination involving a hole coming from the next-highest valence band separared from the top by spin-orbit (SO) splitting. This gives us a value of 4.7 meV for the SO splitting due to the hole in the N-BE, comparable to the values observed in other hexagonal polytypes. This energy can also be obtained from the Arrhenius plot the intensity ration of the lines, Q_0/Q_1 and R_0/R_1.

Summary

Photoluminescence of 8H-SiC polytype is reported from 10 µm thick N-doped epilayers. Three nitrogen non-phonon bound exciton lines are observed together with their phonon replicas; one NP line is thus missing to complete the spectrum. In addition free-exciton phonon replicas are seen which allows the determination of the excitonic band gap at 2792 meV. The ionization energies of the three nitrogen donors are deduced to be 53, 74 and 90 meV, respectively.

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