

Several investigations have documented that dislocations in silicon give rise to characteristic photoluminescence (PL) spectra below the band edge. First showed in [3] which labeled them D1 (0.812eV), D2 (0.875eV), D3 (0.934eV) and D4 (1.000eV). The samples were deformed at 850° C by bending, so that dislocation densities were inhomogeneous along the samples. [3] states that the intensity of these lines increases when the dislocation-rich parts of the crystal are approached. At the same time the intensity of the intrinsic characteristics decreases. The distance between D1-D4 ( $62 \pm 3$  meV) corresponds to the energy of the optical phonons in silicon [3]. [3] reports D1 and D2 are dominant in heavily deformed Si crystals, while D3 and D4 predominate in weakly deformed Si. A similar result was also reported by [8] for small angle grain boundaries using cathodoluminescence.

[9] suggest that D1-D4 are due to dislocations which have been frozen in under low-shear stress. Photoluminescence under uniaxial stress shows that D1/D2 originate in the tetragonal defect with random orientation relative to  $\langle 100 \rangle$  directions. [9] conclude that D3 and D4 are closely related, whereas the independent D1/D2 centers might be deformation-produced point defects in the strain region of dislocations. New lines D5 and D6 emerge when high-temperature, low-stress deformation is followed by low-temperature, high-stress deformation. [9] propose that line D5 is due to straight dislocations and D6 is due to stacking faults. [9] also suggest that D3/D4 photoluminescence is much more characteristic of the dislocations themselves than the D1/D2 emission lines.

The origin of D1 and D2 is not clear. It has been argued that they originate in electronic transition at the geometrical kinks on dislocations [12], point defects [9] and impurities [5] and/or from the reaction products of dislocations [10]. On the other hand, D3 and D4 lines are generally thought to be related to electronic transition within dislocation cores [7]. In addition, it has been suggested that the D3 line most likely is a phonon-assisted replica of D4 [7].

Both [3] and [9] studied plastically deformed silicon made by the Czochralski process (Cz-Si). [16] studied dislocations in multicrystalline silicon (mc-Si) and found similar lines with the entire set of D-lines shifted with around 10meV, presumably due to a strain field. Using a laser annealing technique [11] to introduce dislocations on a Cz-Si wafer, confirm the band location of D1-D4 from [9] in [16]. A principal difference between dislocation D'-lines in mc-Si versus D-lines in Cz-Si is a substantial broadening (60-70meV at 77K) of the D1'/D2' lines [16].

Cz-Si [3]	D1 0.812eV	D2 0.875eV	D3 0.934eV	D4 1.000eV
mc-Si [16]	D1' 0.80eV	D2' 0.89eV	D3' 0.95eV	D4' 1.00eV

Table 1: Energy positions of dislocation D-lines in Cz-Si and D' bands in mc-Si

[16] reveal a linear dependence of the band-to-band photoluminescence intensity and minority carrier lifetime across entire multicrystalline-Si wafers. Photoluminescence mapping in [16] of the 0.78eV (0.8eV) band intensity reveal a linkage to areas of a high dislocation density. This band should also be visible in room temperature [16].

[17] later found that if the contamination level is too low, or too high (dislocation decorated by metal silicate precipitates) the defect photoluminescence band vanished in room temperature. However, a relatively low contamination level of dislocations, in the order of 10 impurity atoms per micron of the dislocation length produces distinguishable defect band luminescence [17].

Dislocation related lines (D-lines) has been observed in low temperature photoluminescence spectra from the regions which included the intragrain defects [14]. They also conclude that grain boundaries are not active recombination centers. [14] also show a TO-phonon replica of the boron bound exciton at 1.093eV. Intensity of boron bound exciton from the long lifetime regions was higher than that from the short lifetime regions. D-lines reported by [9] are in a short lifetime region. For a long lifetime region, [14] observe a peak at 1.00eV which is not the D4 line, but the zonecenter optical phonon sideband of the two-hole transition in the boron bound exciton [2]. There have been no reports on the D-line spectrum missing only the D1 line [14].

[13] study origins of the defects by low temperature photoluminescence spectroscopy, electron backscatter diffraction pattern measurement and the etch-pit observation, and conclude that defects are metal contaminated dislocation clusters which originated from small angle grain boundaries.

## 0.1 Impurities

Diffusion of transition metals into silicon crystals result in a variety of different electrically active levels in the forbidden bandgap.

Copper doping of silicon crystals results in an intense emission at 1.014eV [?]. [?] introduce Fe atoms into a float-zone silicon crystal and observe a spectrum of 0.735eV which relate to a complex defect containing iron.

Silicon samples containing chromium-boron pairs exhibit characteristic luminescence lines in the 0.84eV region where the intensity increased linearly with laser power [?]. [?] observe a luminescence spectra around 1.07eV in boron-doped, iron-diffused crystalline silicon and suggest the source is B-Fe pairs.

Investigation in [4] show that transition-metal contamination plays an important role in the production of D-band luminescence from silicon samples containing either epitaxial stacking faults or oxidation-induced stacking faults. However, [10] later concluded that metallic impurities don't seem to be related to D1 and D2 luminescence.

Room temperature mapping of the 0.77eV band is attributed to oxygen precipitates in thermally treated silicon made by the Czochralski process (Cz-Si) [15]. This band peak shifts parallel to the bandgap with temperature. The increase of this band on the dislocation lines is due to the preferential precipitation of oxygen [15].

[6] state that the deep-level emission from multicrystalline silicon with an intensity maximum at 0.78eV at room temperature is different from that of the D1 line at low temperature. Furthermore, [6] suggest that the 0.78eV emission is associated with oxygen precipitation, and that the intra-grain defects are dislocation clusters decorated with oxygen impurities in addition to heavy-metal impurities.

Iron images in [?] reveal internal gettering of iron to grain boundaries and dislocated regions during ingot growth.

Abbreviation	Description
$B_{TO}$	TO phonon replica of the Boron bound exciton [13]
$D_a$	Broad background emission [15]
$D_b$	Oxygen impurity band [15]
CZ-Si	Czochralski processed Silicon
D1	Dislocation related line 1 [3]
D1'	Dislocation related line 1 for mc-Si [16]
D2	Dislocation related line 2 [3]
D2'	Dislocation related line 2 for mc-Si [16]
D3	Dislocation related line 3 [3]
D3'	Dislocation related line 3 for mc-Si [16]
D4	Dislocation related line 4 [3]
D4'	Dislocation related line 4 for mc-Si [16]
EBIC	Electron beam induced current [1]
EBSP	Electron Backscatter Diffraction Pattern [13]
FZ-Si	Float-zone silicon
EFG	Edge-define Film-fed Growth
mc-Si	Multicrystalline silicon
R1BB	One phonon replica of band edge emission [1]
R2BB	Two phonon replica of band edge emission [1]
SA GB	Small Angle Grain Boundary
ZPL	Zero Phonon Line [?]

Table 2: Abbreviations

D1 and D2: It has been argued that they originate in electronic transition at the geometrical kinks on dislocations [12], point defects [9] and impurities [5] and/or from the reaction products of dislocations [10].

D3 and D4 lines is generally thought to be related to electronic transition within dislocation cores [7]. In addition, it has been suggested that the D3 line most likely is a phonon-assisted replica of D4 [7].

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## A Silicon energy bands

Energy	Name	Temp.	Impurity / Defect	Observed in
0.735eV	ZPL	22K	Fe contamination	[?]
0.76-0.8eV	Defect	290K	Dislocation with low contamination	[16] [17]
0.77-0.78eV	D <sub>b</sub>	4.2-295K	Oxygen impurity band	[15] [6]
0.780eV	CrB <sup>0r</sup>	4.2K	CrB <sup>0</sup> phonon replica	[?]
0.80eV	D1'	77K	Dislocations	[16] [17]
0.812eV	D1	4.2K	Dislocation related line	[3] [9] [1]
0.8160	CrB <sup>2</sup>	4.2K	Cr-B excitation of local vibrations	[?]
0.8402	CrB <sup>1</sup>	4.2K	Cr-B excitation of local vibrations	[?]
0.8432eV	CrB <sup>0</sup>	4.2K	Cr-B pair no-phonon	[?]
0.875eV	D2	4.2K	Dislocation related line	[3] [9] [1]
0.89eV	D2'	77K	Dislocations	[16] [17]
0.8-0.9eV	D <sub>a1</sub>	11K	Broad background emission under D1/D2	[15]
0.934eV	D3	4.2K	Dislocations	[3] [9] [1]
0.95eV	D3'	77K	Dislocations	[16] [17]
0.953eV	D5	4.2K	Straight dislocations	[9]
0.98eV	R2BB	80K	Two phonon replica of band edge emission	[1]
0.9-1.0eV	D <sub>a2</sub>	11K	Broad background emission under D3/D4	[15]
1.000eV	D4	4.2K	Dislocations	[3] [9] [1]
1.00eV	D4'	77K	Dislocations	[16] [17]
1.014eV	Cu <sub>0</sub>	4.2K	Copper doping	[?]
1.0089eV	FeB <sup>0</sup> (TO)	Fe-B pair phonon replica [?]		
1.0126eV	D6	Stacking faults		[9]
1.04eV	R1BB	80K		One phonon replica of band edge emission
1.0504eV	FeB <sup>2</sup>	Fe-B pair contamination		[?]
1.0595eV	FeB <sup>1</sup>	Fe-B pair contamination		[?]
1.0692eV	FeB <sup>0</sup>	6K		Fe-B pair no phonon
1.092eV	BE1	4.2K		Bound exciton
1.093eV	B <sub>TO</sub>	4.2K		TO phonon replica of Boron bound exciton

Table 3: Silicon energy bands

Ref.	Sample type	Excitation process	Pro-	Area	Processing	Doping
[13]	mc-Si	532nm Nd:YVO <sub>4</sub>		0.1mW/10 $\mu$ m diameter	Sawing damage etched by HNO <sub>3</sub> /HF	B-doped
[15]	Cz-Si	Kr ion laser 647nm		10 $\mu$ m		Undoped
[3]	Cz-Si	Xenon lamp		50mW on 3mm modulated at 9Hz	deformed by bending at 850° C	undoped, weak n and p
[16]	mc-Si	800nm AlGaAs laser		Pulsed 300mW / 3mm	surface	Produced by block-casting technique for Baysix
[17]	mc-Si	800nm AlGaAs at 140mW			Produced by EFG	
[1]	mc-Si and FZ-Si	Ar ion 514nm at 300mW		100 $\mu$ m	Produced by EFG	boron doped $10^{15}cm^{-1}$
[9]	FZ-Si	Kr-ion 647nm, Ar-ion 415nm and Nd-YAG 1064nm			Deformed a 650° C and 850° C	residual $10^{12}cm^{-3}$ boron
[6]	mc-Si	Nd:YVO 532nm		6mW, 10 $\mu$ m diameter	Slicing damage etched off by HNO <sub>3</sub> /HF	boron doped
[?]	FZ-Si and CZ-Si			50mW laser	Etched with HNO <sub>3</sub> /HF. Chromium diffused	boron doped
[?]	FZ-Si	Ar+ 514nm		500mW	Fe diffused	boron doped
[?]	FZ-Si	Argon laser			Fe diffusion	undoped
[?]		Ar+ 514nm at 1.5W				Cu doped

Table 4: Sample types