STUDY OF THE OXYGEN-RELATED PHOTOLUMINESCENT (1096.9 meV) CENTRE IN NEUTRON-IRRADIATED CZ-Si. FORMATION AND STRUCTURE

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•INTRODUCTION

• Oxygen-related centres formed in Czochralski (CZ) Silicon have been object of intense investigation since the discovery of thermal donors (TD).

• The formation processes of such centres of marked technologically interest has increased the activity in the research field of radiation damage by neutron, electron or ion bombardment as an efficient way of creating new defect centres in silicon.

• The study of simple centres created after annealing in irradiated crystals during the first stages of the TD formation can provide useful information to reveal the structure of these centres

•OBJECTIVE

• Investigate a new oxygen-related photoluminescence (PL) centre in Silicon formed in neutron-irradiated CZ-Si after thermal annealing at 350-400 ºC

Formation processes, structure and composition

INTEREST

• The investigated centre is an important PL centre created after annealing in irradiated in CZ- Si.

• The PL line of this centre at 1096.9 meV together with the PL-line of the I1 centre (neutral divacancy?) at 1018.2 meV are the major features of the PL spectra of neutron-irradiated CZ-Si annealed between 100-350 ºC.

• The PL-line arises from the emission of a binding exciton to the centre.

• The low activation energy for bound exciton dissociation suggests that the centre is presumably related to a shallow iso-electronic centre.

• The structural characterization is useful to understand the chemical processes involved in the formation of the centre.

• The centre is passivated neither by Li nor by H

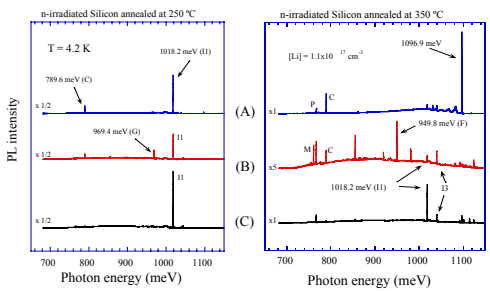
•METHOD:

- FT Photoluminescence spectroscopy
- Isotope structure
- PL temperature dependence
- Uniaxial stress measurements

Spectroscopic data of the 1096.9 meV-line centre:

Exciton binding energy:	1155.4 - 1096.9 = 58.5 meV
Activation energy:	ΔE = 5.1 meV
Resonant TA mode energy:	ħω= 14.1 meV
Huang-Rhys factor:	1.35
Exciton relaxation energy:	S <ħω> = 31 meV
Oxygen isotopic ZPL-shift:	$E_{ZPL}(^{18}O) - E_{ZPL}(^{16}O)$ = +0.037 meV
centre symmetry:	Monoclinic I

CENTRE FORMATION



PL spectra at 4.2 K of

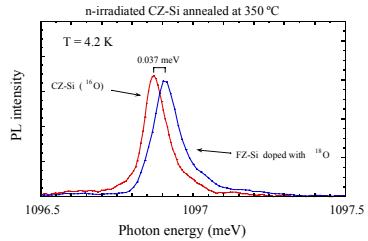
(**A**) **CZ-Si** [O]=2x10^{18} cm^{-3}, (**B**) **FZ-Si** with [C]= 1.6x10^{17} cm^{-3}, and (**C**) carbon- and oxygen-lean **FZ-Si**, neutron-irradiated with a dose of 1x10^{17} cm^{-2} and annealed at 250 and 350 ºC for 30 minutes.

[Li] = 1.1x10^{17} cm^{-3} for the three samples.

Note the different intensity magnification for each spectrum.

Spectral resolution: 0.25 meV

OXYGEN ISOTOPIC SHIFT

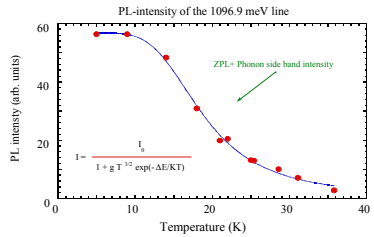


Isotope shift of the 1096.9 meV Zero-phonon line (ZPL) at 4.2 K.

The high resolution spectra correspond to **1)** CZ-Si with [^{16}O] = 2x10^{18} cm^{-3}, and to **2)** FZ-Si doped with [^{18}O] = 4.1x10^{17} cm^{-3}, [^{16}O] = 1.7x10^{17} cm^{-3} and [C] = 7x10^{15} cm^{-3}, neutron irradiated with a dose of 1x10^{17} cm^{-2} and annealed 390 ºC for 30 minutes. [Li] = 2x10^{16} cm^{-3}

Spectral resolution: 0.012 meV.

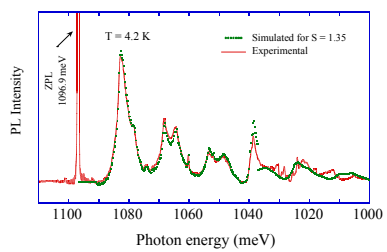
ACTIVATION ENERGY: VARIATION OF THE PL-INTENSITY WITH TEMPERATURE

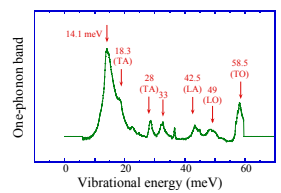


Variation of the PL-line intensity with temperature.

The fitted curve corresponds to I_o= 57, g = 0.27 K$^{2/3}$ and an activation energy for bound exciton dissociation: ΔE = 5.1 meV

ELECTRON-PHONON COUPLING: PHONON SIDE BAND ANALYSIS





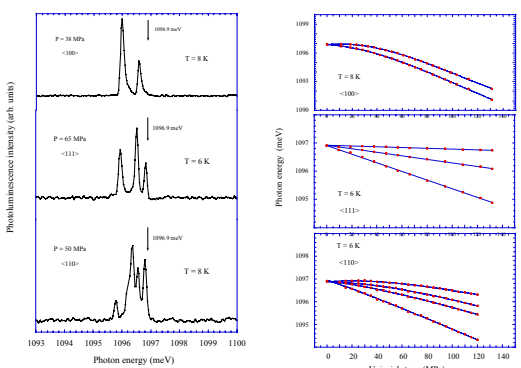
Note the strong electron-phonon coupling provided by resonant TA modes around 14.1 meV

One-phonon contribution.

Peak labelling represents the phonon energy of maxima of the phonon state density, and the associated phonon branch

Simulated spectrum up to five-phonon contributions with a Huang-Rhys factor, S = 1.35.

CENTRE SYMMETRY: UNIAXIAL STRESS MEASUREMENTS



•CONCLUDING REMARKS

• There is a correlation between the two major PL lines observed in CZ-Si:

anneal out of I1 ⟶ formation of the 1096.9 meV PL line centre.

• The centre responsible for the 1096.9 meV PL line is presumably formed by complexing the trigonal I1 centre with oxygen.

• The presence of I1 (1018.2 meV) in the PL spectrum of the C-rich FZ-Si supports the divacancy model as centre responsible for the this line

• Proposed model : *an oxygen-vacancy iso-electronic centre*