High sensitivity infrared absorption spectroscopy and infrared defect dynamics of silicon crystal (17) Various nitrogen states, STD and multiple absorption peaks

シリコン結晶の高感度赤外吸収と赤外欠陥動力学（17）窒素の各種状態、STDと複ピーク

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Introduction Nitrogen in silicon usually forms interstitial pair (N_iN_i) and its concentration is measured by the infrared (IR) absorption by the pair complexes (NNO_n, n = 0-2). Also it is known that N in CZ silicon at low concentrations forms shallow thermal donor (STD) of NO pair complexes (NO_n, n = 1-4) [1]. We found the infrared absorption for the local vibration modes (LVM) of STD at 1002, 973 and 855 cm^{-1} [2, 3] and identified the origin to be O(NO)O [4,5]. It was supported by the calculation [6]. Furthermore, we found that the absorption line at 551 cm^{-1} decreased after the electron-beam irradiation and the 688 cm^{-1} line appeared by the post annealing at 400 °C in FZ silicon [7], and assigned the latter as VVNN [8] which was predicted theoretically [9]. We assigned 551 cm^{-1} line as N_i and found 689cm^{-1} in as-grown FZ crystal and assigned as VN_s [10]. Here we add $(ONO)O_n$ to construct 7 STD structure models. Multiple absorption peaks were reported.

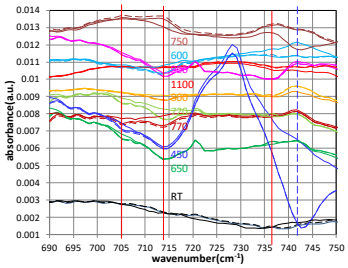
#	year	stucture	LVM wavenumber (cm^{-1})	process	character
1	1959	N_s	653	implantation	low electronic activity
2	1981	$(NN)O_n$	766, 801, **810**, 963, 996, **1018**,1027	doping	defect suppression
3	1983	$(NO)O_n$,$(ONO)O_n$	**714**, **763**, **946**, **737**, **1002**, **973**, **855**, ---	grown-in	shallow thermal donor
4	2000	VNN, VVNN	**726**,**778**, **688**	irradiation	grown- in defect
5	2018	N_i,VN_s	**551**, **556**, **689**	grown-in	various states (monomer)

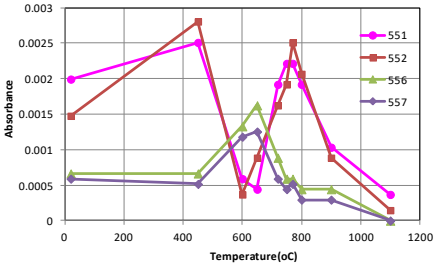
Experimental The samples were N-doped CZ and FZ crystals at various contents. Some of them were irradiated with electron beams and then annealed. The differential IR absorption was measured at a resolution of 2 cm^{-1} for the 2 or 10 mm thick polished samples at room temperature, using the non-doped or non-irradiated sample as the reference. To detect the weak absorption signal the strong background absorption by the NN and NO pair, oxygen and phonon were deleted from the absorption spectrum by using the Lorentzian function fitting.

Results and discussion: STD and multiple peaks More than 7 species of STD have been reported previously [0]. We predicted 4 construction by analogy with NN ring structures, NO, (NO)O, O(NO) and O(NO)O. Gali predicted ONO symmetric double ring as STD [11]. Fujita calculated and assigned 855 cm^{-1} as ONO [6]. Alt determined the number of oxygen [12] and experimentally supported Fujita's 855 cm^{-1} assignment [13]. We add $(ONO)O_n$ (n=0-2) double ring groups for the STD candidates as the diagram shown below:

STD ID	N-O-4, 5, 6	N-O-3	N-O-1, 2	N-O-8	
Composition	NO	NO2	NO3	NO4	
Structure & Reaction	NO ← - O + → (NO)O, O(NO) ← - O + → O(NO)O				NO ring group
		↑↓			
		ONO ← - O + → (ONO)O ← - O + → O(ONO)O			ONO ring group
Temperature	750°C	650 °C	600 °C	600 °C	

Left figure shows the annealing temperature dependence of 714(NO) and 737 (NOO) cm^{-1} absorption. Right figure shows the complementary temperature dependence of the (551, 552, N_i) and (556, 557, N_i+O?) cm^{-1} absorption pairs.





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