High sensitivity infrared absorption spectroscopy and infrared defect dynamics of silicon crystal/ 2-nd generation (26) LVM IR absorption of shallow thermal donor

シリコン結晶の高感度赤外吸収と赤外欠陥動力学/第二世代 (26) シャロ−サーマルドナーの赤外吸収

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In 1968, shallow donors were found in annealed N-doped FZ Si [1]. In 1986, 5 electron transition absorptions were observed in CZ-Si and their thermal behavior was reported [2, 3]. In 1996, two types of models were proposed by a theorist group, (NO) ring (N_i-Si-O_i-Si rectangle, [4]) and (ONO) double ring [5]. In 2001, 1 N inclusion was supported and STD was suggested to be dominant in low N Si [6], although (NN) ring is dominant in high N Si [7]. Sum of two STD absorption at 240 and 250 cm^{-1} was proposed to measure N concentration in low N Si [8].

We examined LVM IR absorption of STD. In 2003, quasi equilibrium among (NN), (NN)O and O(NN)O in annealing was reported [9]. We examined the same annealed samples and found candidates at 714, 736, 841, 855, 862, 941, 945, 973, 1002, 1008, 1065 cm^{-1} in 2004 as shown in Fig. [10]. In 2005, we reported 3 of them at 855, 973 and 1002 cm^{-1} and assigned 973 and 1002 cm^{-1} as O(NO)O from the O(NN)O like thermal behavior [11, 12, 13]. We asked the theorists to calculate LVM. In 2007, they reported the results on (NO), (NO)O and (ONO), and assigned the observed 973 and 1002 cm^{-1} as (NO)O and 855 cm^{-1} as (ONO) [14].

The problem arose, 973 and 1002 cm^{-1} absorption behavior suggests 2 O accompanying with (NO) and 855 cm^{-1} accompanies at least 1 O. (ONO) must be largest at 800 ºC, conflicting with the observed thermal behavior.

We composed 5 models for STD; (NO), (NO)O, O(NO), O(NO)O and (ONO). We took care (1) N-O-3 at 240 cm^{-1} and N-O-4, 5 at 242 and 250 cm^{-1} remain after annealing at 800 ºC, suggesting no O accompanies. (2) Thermal behavior of N-O-3 deflects around 600 ºC [2, 3]. We interpreted it due that there are low-T type and high-T type. For (2), we examined absorption around 855 cm^{-1}. Previously observed 840 and 862 cm^{-1} absorption (Fig.) shows peak at 800 ºC. Therefore, we concluded that 855 and 1065cm^{-1} absorption comes from O(NO) and 840 and 863 cm^{-1} from (ONO).

For (1), We examined high-T absorption at 714 cm^{-1}. In 2018, we reported it from irradiated and annealed O-rich NFZ samples and named it 800 ºC group [15]. It must be (NO) originated. (NO)O absorption is left. It may locate at 10-20 cm^{-1} higher frequency. 739cm^{-1} absorption is the candidate. Like other absorption it overlaps the strong phonon bands, making analysis difficult. Table summarizes the identification of STD LVM IR absorption bands and correspondence with electron transition. There are low-F H_2O type and high-F BF_3 type LVM for all STDs. More absorption will be assigned.

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(NO)Om	Comp.	LVM	STD	(NN)Om	Tmax
NO	NO	714[1,2]	N-O-4,5 242, 250	(NN) 766,963	800
(NO)O	NO2	739[1]	-	(NN)O 801,996,1027	600
O(NO)	NO2	855, 1064[1]	N-O-3 240	ibid	600
(ONO)	NO2	840[1], 862[1]	N-O-3 240	ibid	800
O(NO)O	NO3	973, 1002	N-O-1,2 234, 237	O(NN)O 810, 1018	600