Optical Property modifications of sapphire and diamond

朴在元， 李在桑，李燦榮

Jae-Won Park, Jae-Sang Lee, Chan-Young Lee

Korea Atomic Energy Research Institute, Daejeon, South Korea

(要約2～3行)

The density of green color of diamond produced by proton irradiation is dependent on its inherent color. Mn ion implantation into colorless sapphire did not turned any color, but the light-brown color appears after annealing in the air.

キーワード: Proton irradiation, Ion implantation, Optical property

１．目的

Modification of optical properties of sapphire and diamond by implanting Mn and proton (H+) elements respectively and subsequent heat treatment aimed to apply for the coloration when used as gemstones and for the optoelectronic applications as thin films.

２．方法

100 keV Mn^+ ions from 400keV ion accelerator were implanted into colorless sapphires with a dose of about 1×10^{17} ions/cm^2 and 2MeV H^+ ions using 3MV Tandem accelerator were implanted into diamonds with a dose of about $2\text{-}3\times10^{16}$ ions /cm^2. Post-irradiation annealing were conducted at 950℃ in air for sapphire for 5 hours. First-principles density-functional theory (DFT)[1] calculations were done to predict the band gap variation of the Mn sapphire.

３．研究成果

Fig. 1 is a photo of green colored diamonds produced by 2MeV proton (H^+ ion) implantation with a dose of $2\text{-}3\times10^{16}$ ions/cm^2. The original colors of the diamond before the irradiation were light brown and this color changes into light green [Fig. 1(a)] and green [Fig. 1(b)]. The difference is not so vivid visually but recognizable only when exposed to a bright light source. We want blue color changed diamond using proton bombardment, but we did not earn the result in this time. So we need to carry out lower dose experiment next time. Further decrease in the proton dose may be required for the color density reduction of the green diamond and for the blue diamond.

Mn ions implantation with a dose of 1×10^{17}ions/cm^2 turned the colorless sapphire into brown [Fig. 2 (b)]. The brown color was turned to light brown after the annealing at 950℃ for 5 hours[Fig. 2 (c)].

Fig.3 shows the calculated results of density of states (DOS) [6] of a white sapphire (a) and Mn doped sapphire (b). This calculation implies that optical property of sapphire is varied depending on the dopant species.

４. 結論・考察

In our previous study, we obtained the reddish color diamond as the result of proton (H^+ ion) irradiation and subsequent annealing at 600℃in vacuum for 2 hours. We thought that the dark green color of proton irradiated diamond resulted from the too large dose of proton and the reduced dose result in the lighter green color in this experiment. We have found the color density is little different in below $3x10^{16}$ ions/cm^2 as observed visually. When a certain impurity atoms are included in a natural diamond, the diamond is colored, for example, a brown colored diamond is due to N impurity. However, a 2 MeV proton irradiation turned the color into green regardless the original color. It seems the darker green diamond is produced as the more impurity exists in the pristine diamond.

Through the implantation of Mn into colorless sapphire we cam expect an appearance of a new color due to the possible band structure modification[1)]. Mn implantation and then subsequent annealing produces brown color, and the brown color changed to the light brown color after the annealing at 950℃ in the air. According to the DOS calculation, Mn doping in sapphire should produce a different color as shown in Fig.3, We are trying to understand this deviation form the expectation.

In summary, a proton-irradiated diamond showed green color emission at below $3\ x10^{16}$ ions/cm^2 and the density of the green color depends on total ion dose. Mn ion implantation into colorless sapphires changed the color into brown but the post-implantation annealing changed the color to the light brown.

５. 引用(参照)文献等

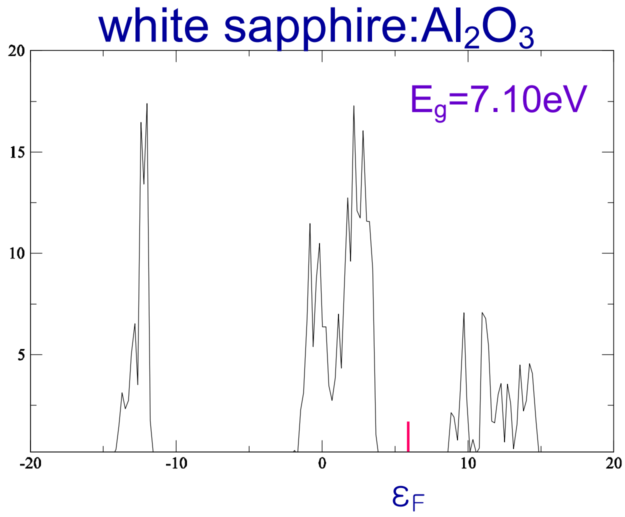
1) J. Y. Lee, J. Park, and J. H. Cho, Appl. Phys. Lett. 87, (2005) 011904

(a) (b)

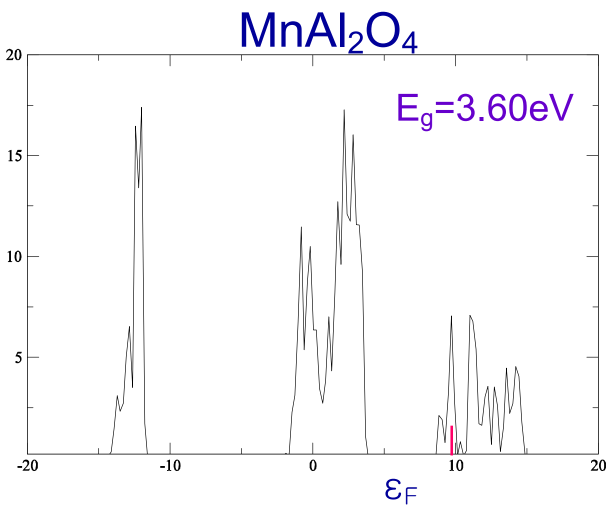
Fig. 1 Photos of green colored diamonds produced by 2 MeV proton implantation with a dose of 2-3×10^{16} ions/cm^2: (a) White brown color changes to light green at 2×10^{16} ions/cm^2. (b) White brown diamond turned into green color at 3×10^{16} ions/cm^2.

(a) (b) (c)

Fig. 2. Mn ion implantation on a colorless sapphire: (a) the prepared sapphire is colorless and transparent. (b) 100 keV Mn ions are implanted onto the colorless sapphire with a dose of 1.0×10^{17} and turn the sapphire brown. (c) the brown color turn to light brown after the annealing at 950℃.



(a)



(b)

Fig. 3. Calculated results of density of states (DOS): (a) white sapphire and (b) Mn doped sapphire doped sapphire. A large underestimation (~20%) of the band gap compared to the experimental value is the well-known shortcoming of the LDA. This calculation implies that optical property of sapphire is varied as a function of the dopant.