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Structural forms of the titanium defects in diamonds of different habitus

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Modern technology of diamond synthesis expands the range of applications for diamond. Therefore doping diamond with different ions to obtain new properties of crystals is very important task. Significant recent progress has been achieved in understanding the occurrence in the diamond structure of transition metal ions with large atomic radii. It is shown that ions of nickel and cobalt incorporated into the diamond structure form a double semivacancy defect with octahedral environment of the ion. In the structure of such a defect metal - carbon length is ~ 2 Å, which is typical of a metal - ligand distance in many complex compounds. Among the natural diamonds the samples with yellow photoluminescence (PL) occupy a special place. The peculiarity of these crystals is the regions with a low content of nitrogen impurity. The X-ray phase analysis of the xenolith sample being the growth medium for a large number of diamond crystals under study, as well as of inclusions in these diamonds identified an abnormally high content of titanium compounds. Our comprehensive studies showed that the features of the crystals are three types of nitrogen-titanium centers. EPR and PL data show that the centers OK1/S1, N3/440.3 nm and NU1 have the structure of the double semivacancy centered on the titanium ion with one nitrogen in the first coordination sphere, the nitrogen-titanium pair in neighboring carbon positions, and the split <100> nitrogen-titanium interstitial configuration respectively. The NU1 center occurs in the PL spectrum as a vibronic system with a zero phonon line at 485 nm. The phonon energy analysis of the N3/440.3 nm and NU1 centers confirms the presence of titanium ion in their structure. High temperature-high pressures annealing (2000 C, 7 GPa) showed that the centers are stable at these conditions and can not be transformed into each other. Previous radiographic analysis has shown that titanium occupies predominantly cubic growth sector of the crystal. To clarify the peculiarities of the formation and the distribution of nitrogen-titanium centers a number of diamond crystals of different habitus containing nitrogen-titanium centers have been studied. The specimens under study were the crystals isolated from the xenolith abnormally enriched in titanium compounds, cubic crystals of the Yakutiyan northern placers and various crystals of mixed growth. These studies showed that the diamonds of cubic habitus is characterized by the formation of a center OK1/S1 having a structure of a double semivacancy. N3/440.3 nm and NU1 nitrogen-titanium centers are typical of the diamonds of octahedral and mixed habitus. It is assumed that titanium impurity in a cubic sector transforms into the double semivacancy structure, which captures the nitrogen atom forming a center OK1/S1. Studies on the diamond crystals synthesized with titanium in the growth medium as a nitrogen getter and later annealed showed that the N3/440.3 nm center is formed in the process of the diffusion and interaction of nitrogen impurity with titanium ions in the substitutional position. The center NU1 seems to be also a result of the interaction of the titanium impurity with interstitial nitrogen. It is likely the peculiarities of the occurrence of nitrogen-titanium centers in the diamond crystals of cubic, octahedral and mixed cubo-octahedral habitus are due to diverse ratios of nitrogen and titanium impurities in different growth sectors.