Characterization of Heating and Nitriding Processes of Titanium Thin Films Grown on NaCl (001) Substrate Held at Room Temperature*

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Both hcp-Ti and CaF$_2$-type TiH$_x$ ($x \approx 1.5$) with preferred orientations have been grown in as-deposited Ti films on NaCl (001) substrates held at room temperature (RT). In order to clarify atomistic growth processes of TiN$_x$ films due to the implantation of nitrogen ions (N$^+$) with 62 keV into Ti films, changes of the crystallographic and electronic structures of Ti thin films by heating and by nitriding during N-implantation were investigated by in-situ transmission electron microscope (TEM) observations combined with electron energy loss spectroscopy (EELS), with the aid of molecular orbital calculations. H atoms which constituted TiH$_x$ in the as-deposited Ti films were released with heating up, and were completely released at 350°C. The H-released unstable fcc-Ti sublattice was then epitaxially transformed into hcp-Ti. The loss peak observed by EELS for TiH$_x$ shifted to the lower energy side with the decrease in the electron density in the hybridised valence band due to the release of H atoms from TiH$_x$ during heating. On the other hand, the TiN$_x$ was epitaxially formed by the N-implantation into the hcp-Ti, through the transformation of the hcp-Ti to fcc-Ti sublattice, partially inheriting the atomic arrangement of the hcp-Ti and accompanying the occupation of O-sites of the fcc-Ti by N atoms. The loss peak during N-implantation into the hcp-Ti films gradually shifted to the higher energy side with the increase in dose, due to the increase in the electron density in the hybridised valence band. Taking into account the bonding interaction of Ti sublattices due to the transformation mechanism between fcc-Ti sublattices and hcp-Ti sublattices due to the release of H atoms or due to the implantation of N atoms will be clarified. [DOI: 10.1380/ejssnt.2009.625]

Keywords: Ion-implantation; TiH$_x$; TiN$_x$; fcc-hcp transformation; in-situ TEM

I. INTRODUCTION

Titanium nitrides, TiN, formed by various techniques such as ion implantation, ion beam assisted deposition, magnetron sputtering, physical vapor deposition (PVD) and chemical vapor deposition (CVD), are non-stoichiometric compounds and show covalent properties as well as metallic and ionic properties, which make them fascinating for both fundamental research and technological applications [1–11]. Their fascinating properties are naturally related to the crystallographic and electronic structures. Due to the covalent properties [2, 9–11], the nitrides of Ti are technologically useful as, for instance, corrosion resistant coatings on cutting tools and diffusion barriers in silicon microcircuits [3–8]. It has been revealed that the interesting physical properties are related to the crystallographic (preferred oriented) and electronic structures, and that some properties of epitaxially grown TiN films are superior to those of polycrystalline ones. Thus, much interest has been focused on the epitaxial films and the atomistic interfacial structures between TiN films and substrates [4, 6–11]. Recently, it was reported through ex-situ experiments that NaCl-type TiN$_x$ films were “epitaxially” grown by N-implantation into epitaxially deposited Ti films held at room temperature (RT) [12–14]. However, atomistic growth processes of TiN$_x$ films due to ion implantation, and changes of the crystallographic and electronic structures of Ti thin films by heating and by nitriding during N-implantation have not been sufficiently studied.

The purpose of this work is to study changes of the crystallographic and electronic structures of Ti films by heating and by nitriding during N-implantation into Ti films, using in-situ transmission electron microscope (TEM) equipped with the instrument for electron energy loss spectroscopy (EELS), and then to clarify the atomistic nitriding processes of Ti thin films due to the N-implantation with the aid of self-consistent charge discrete variational Xα (DV-Xα) molecular orbital (MO) calculations. The present calculations throw light on the hcp-fcc transformation mechanism between fcc-Ti sublattices and hcp sublattices due to the release of H atoms or due to the implantation of N atoms, taking into account the bonding
interaction of Ti sublattices with ligand H or N atoms.

II. EXPERIMENTAL

Titanium films of 100 nm in thickness were deposited on thermally cleaned NaCl (001) surfaces held at RT by an electron beam heating method in an ultra high vacuum. Detailed descriptions of the preparation method for deposited Ti films were presented in earlier papers [12–14]. The Ti films separated from NaCl substrates were heated up to 350°C at a heating rate of 2°C/min in a 400 kV TEM combined with ion accelerators at JAERI-Takasaki [15]. The implantations of N\textsuperscript{+} ions with 62 keV into Ti films held at 350°C or RT were performed in the TEM at an angle of 30° to the surface normal. According to a Monte Carlo simulation using the SRIM2003 code, the projected range of N\textsuperscript{+} ions with 62 keV was 55 nm. Thus, most of the implanted ions are to be retained in Ti films. The N-concentrations in Ti films were evaluated from the implantation dose measured by a Faraday cage. The maximum dose in this experiment was 5.40 × 10\textsuperscript{17} ions/cm\textsuperscript{2}, which corresponded to the N/Ti ratio of 0.954. The N/Ti ratios indicate the average atomic concentration of implanted N atoms with respect to Ti atoms in the films. The method of DV-Xα MO calculations for investigation of the electronic structures of hcp-Ti, TiH\textsubscript{x} and TiN\textsubscript{y} has been given elsewhere [16].

III. RESULTS AND DISCUSSION

Figure 1 shows typical electron diffraction (ED) patterns taken from (a) the as-deposited Ti film held at RT, (b) the Ti film held at 350°C, and (c) the N-implanted Ti film (N/Ti=0.954) held at 350°C.

FIG. 1: Typical ED patterns taken from (a) as-deposited Ti film at RT, b) Ti film held at 350°C, and (c) N-implanted Ti film (N/Ti=0.954) held at 350°C.
containing TiHₓ crystallites induced the release of H and made TiHₓ crystallites unstable. Furthermore, the H-released unstable TiHₓ (fcc-Ti sublattice) absorbed implanted N atoms to maintain the fcc-Ti sublattice, and the occupation of O-sites of the H-released fcc-Ti sublattice by implanted N atoms led to stabilization of the unstable fcc-Ti sublattice. These processes resulted in the formation of stable crystallites, (110)-oriented TiNₓ, not of hcp-Ti. The (001)-oriented TiNₓ was mainly formed by the transformation of the (03 • 5)-oriented hcp-Ti to (001)-oriented fcc-Ti, accompanied by the occupation of O-sites of the fcc-Ti sublattice by N atoms. These results agree with those of the previous ex-situ experiments [12–14].

The orientation relationship between (03 • 5)-oriented hcp-Ti and (001)-oriented fcc-Ti, which is the Ti sublattice of TiNₓ, is shown in Fig. 2. The closed circles represent Ti atoms. The (001)-oriented TiNₓ are epitaxially formed by the transformation of (03 • 5)-oriented hcp-Ti sublattice to (001)-oriented fcc-Ti sublattice during the N-implantation, inheriting the square EFJK and the octahedron GEFJKL in Fig. 2(a) as well as by the occupation of O-sites of the (001)-oriented fcc-Ti sublattice by N atoms. The shaded square EFJK in Fig. 2(a) is the (03 • 4) plane. A dihedral angle of the (03 • 4) plane and (03 • 5) plane which is parallel to the substrate surface is about 6.2°. Therefore, the former also is nearly parallel to the substrate surface. In order to obtain an fcc-Ti structure as shown in Fig. 2(b), the B atom in Fig. 2(a) has to be shifted to the center of gravity of the triangle ABQ. The shifted B atom is represented by the open circle labeled as B*. Open circles labeled as alphabetical letters with asterisks in Fig. 2(a) represent Ti atoms shifted in the same way that the B atom shifted to the B* atom. This transformation induced by the shear on the (00 • 1) plane containing A-D atoms in Fig. 2(a) leads to the formation of the fcc structure shown in Fig. 2(b). It should be noted that the square EFJK and the octahedron GEFJKL in Fig. 2(a) correspond to those in Fig. 2(b) and are preserved in this hcp-fcc transformation. In this transformation, the inheritance of the square EFJK and/or the octahedron GEFJKL in Fig. 2(a) plays a prominent role in the epitaxial formation of the fcc-Ti sublattice. This hcp-fcc transformation processes of the Ti sublattices are the reverse processes of the transformation of the H-released fcc-Ti sublattice into hcp-Ti; in order to obtain the hcp-Ti structure in Fig. 2(a), the B atom, which corresponds to the open circle labeled as B* in Fig. 2(a), has to be shifted to the center of gravity of the triangle BCN in Fig. 2(b). The shifted B atom is represented by the solid circle labeled as B in Fig. 2(a). The shift of open circles labeled as alphabetical letters with asterisks in Fig. 2(a), in the same way that the B* atom shifted to the B atom as mentioned just above, results in the formation of the hcp structure. In other words, this transformation induced by the shear on the (111) plane containing A-D atoms in Fig. 2(b) leads to the formation of the hcp structure shown in Fig. 2(a). These atomistic epitaxial transformation mechanism of the H-released fcc-Ti sublattice into hcp-Ti and of the N-implanted hcp-Ti into TiNₓ (fcc-Ti sublattice) will be explained in detail later.

Figure 3 shows the variation of energy loss spectra with the increase in temperature of the films. Figures 3(a) and 3(b) show the electron energy loss spectra obtained from the area of TiHₓ as shown by a large arrow in Fig. 1(b) of the previous paper [14], and from the area where hcp-Ti grow outside the band-like contrast region, respectively. The loss peak (≈ 47 eV) denoted by the line of Ti 3p-3d corresponds to the Ti 3p-3d resonant photoemission [17], in which an electron is excited from the Ti 3p state to an empty Ti 3d state and then an electron relaxes back to the Ti 3p state, and another electron of Ti 3d states is ejected. It should be noted that the positions of Ti 3p-3d peaks are almost invariant with increasing the tempera-
tecture in this experiment, as seen in both Figs. 3(a) and 3(b). This means that the energy of core levels is almost invariant with the temperature. Therefore, inspection of the energy loss due to the excitation of plasmon shown in Figs. 3(a) and 3(b) gives us the information on the bonding character between Ti and ligand H or N atoms and on the electron density of conduction and/or valence bands. Analysis of EELS spectra elucidated that the energy loss peak of $\sim 17.0$ eV, indicated by a solid triangle in Fig. 3(b), was ascribed to excitation of plasmon for hcp-Ti. The energy loss of $\sim 17.0$ eV, indicated by a solid triangle for hcp-Ti at RT in Fig. 3(b), was found to agree well with the theoretical value, $\sim 17.6$ eV, of the energy loss due to excitation of plasmon, calculated with the assumption that 3d and 4s electrons are all free [18]. For TiH$_x$, in Fig. 3(a), the energy loss peak of $\sim 19.5$ eV, indicated by a solid triangle at RT, is due to excitation of plasmons by electrons in the valence band consisting of bonding states formed by Ti 3d-4p and H 1s orbitals, which is in agreement with the energy loss reported by Thomas [19]. The higher loss energy for TiH$_x$ than for hcp-Ti at RT can be considered to reflect the existence of additional electrons from H atoms, which result in an increase in the electron density of the hybridized band of Ti 3d-4p and H 1s orbitals. The energy of the loss peaks indicated by solid triangles for TiH$_x$ in Fig. 3(a) shifts to lower energies with increasing film temperature, while there is no shift among the loss peaks indicated by solid triangles for hcp-Ti in Fig. 3(b). This means that the electron density in the valence band consisting of Ti 3d-4p and H 1s bonding states decreases with the release of H atoms from the TiH$_x$ due to the increasing in film temperature. Thus, it is considered that the excitation of electrons of Ti 3d-4p and H 1s bonding states to the antibonding states has been induced by heating the TiH$_x$ up to 100-150°C, and that the increase in the number of phonons by heating also contributes to make the excitation of electrons of the bonding states to the antibonding states easy.

Figure 4 shows the variation of energy loss spectra with the dose of N-implantation into hcp-Ti at 350°C. The energy loss peaks due to plasmon excitation indicated by solid triangles gradually shifted to higher energies with increasing dose. This means that the number of N atoms bonding to Ti atoms increases, and that the electron density in the valence band hybridized by N 2p and Ti 3d-4p states increases gradually with increasing N dose. The peaks of the energy loss of 24.5 eV for N/Ti=0.95 in Fig. 4 were similar to the energy loss of 24.9 eV due to excitation of plasmon for TiN, reported by Pfüger, et al [1]. Therefore, it can be considered that the electron density of the present TiN$_y$ is also similar to that of the TiN$_y$ ($y \geq 0.9$), referring to the results of Pfüger, et al [1]. The loss peak ($\sim 16.0$ eV) denoted by the dotted line connected to the solid square becomes noticeable at N/Ti$\leq 0.38$. This peak is considered to be due to excitation of N 2s electrons to the conduction band [5].

In order to elucidate the atomistic epitaxial transformation mechanism of the H-released fcc-Ti sublattice into hcp-Ti sublattice and of the N-implanted hcp-Ti into TiN$_y$ (fcc-Ti sublattice), DV-Xα MO calculations have been performed for mainly four cluster models shown in Fig. 5. The Ti$_{19}$ cluster of Fig. 5(a) corresponds to a part of the hcp-Ti structure. The Ti-Ti distances are taken to be 0.29238 nm, corresponding to those of the ideal bulk crystal structure. Figure 5(b) shows the Ti$_{13}$H$_8$ cluster of CaF$_2$-type structure. The hydrogen atom as indicated by V, for example, occupies the central position, tetrahedral
FIG. 4: Variation of EELS spectra with the dose of N ions. Solid triangles indicate the loss peaks due to plasmon excitation. The energy loss of $\sim 17.0$ eV was found to agree well with the theoretical value of $\sim 17.6$ eV calculated assuming the $3d$ and $4s$ electrons are all free [18]. The loss peak ($\sim 16.0$ eV) denoted by the dotted line connected to the solid square is considered to be due to excitation of N $2s$ electrons to the conduction band.

(T-) site, of the tetrahedron as formed by B, R, C and N atoms in the fcc-Ti sublattice. The Ti-Ti distances are assumed to be 0.31183 nm, corresponding to those of the observed TiH$_x$ in as-deposited Ti films. A Ti$_{19}$N cluster is shown in Fig. 5(c). The nitrogen atom, indicated by G, occupies the central position (O-site) of the octahedron as formed by A-F atoms in the hcp-Ti cluster of Fig. 5(a). The Ti-Ti distances are assumed to be 0.29238 nm, which is the same as those of the Ti$_{19}$ cluster. A Ti$_{14}$N$_{13}$ cluster for NaCl-type TiN is shown in Fig. 5(d). The nitrogen atom as indicated by G, for example, occupies the O-sites of the octahedron as formed by A-F atoms in the fcc-Ti sublattice. The Ti-N distances are assumed to be 0.21200 nm, corresponding to those of the bulk crystal structure of TiN. Removing of all nitrogen atoms indicated by large open circles from the Ti$_{14}$N$_{13}$ cluster results in forming of an fcc-Ti$_{14}$ cluster.

The calculated density of states (DOS) curves for the hcp-Ti$_{19}$ and fcc-Ti$_{14}$ cluster models are shown in Fig. 6. Each curve corresponds to superimposition of Ti $3d$, Ti $4s$ and Ti $4p$ DOS for each model. The line at 0 eV represents the Fermi level, $E_f$. The DOS curve for Ti$_{19}$ has a larger peak indicated by the line “a” just below $E_f$, whereas the DOS curve for the hcp-Ti$_{19}$ shows a larger peak indicated by the line “A” at the lower energy than that of “a”. The energies of peaks of the DOS curve for
TABLE I: Bond overlap populations between Ti atoms, Ti and H atoms, and Ti and N atoms for the employed models.

| Cluster Model | Ti-Ti OP | Ti-N OP | Ti-H OP |
|---------------|---------|---------|---------|
| Ti_{19}       | 0.231   |         |         |
| Ti_{19}N      | 0.135   | 0.277   |         |
| Ti_{19}H_8    | 0.083   |         | 0.184   |
| Ti_{19}N_{13} | 0.042   | 0.289   |         |

TABLE II: Overlap population of each bond between Ti atoms for the Ti_{19}H_8 and Ti_{19}H_7 (without V atom) cluster models in Fig. 5(b).

| Cluster Model | B-S, atoms | B-C, atoms | N-C atoms | B-R atoms |
|---------------|------------|------------|-----------|-----------|
| Ti_{19}H_8    | 0.274      | 0.274      | 0.274     | 0.084     |
| Ti_{19}H_7 (without V atom in Fig. 5(b)) | 0.278 | 0.317 | 0.310 | 0.163 |

The fcc-Ti_{14} indicated by “i”, “c” and “d” are higher than those for the hcp-Ti_{19} indicated by “B”, “C” and “D”. Furthermore, the averaged energies per unit electron density of states under the $E_f$ for the hcp-Ti_{19} and fcc-Ti_{14} clusters in Fig. 6 are $-2.07$ eV and $-1.71$ eV, respectively. These mean that the electronic energy of the fcc-Ti_{14} is higher than that of the hcp-Ti_{19}. Therefore, it is considered that the H-released fcc-Ti becomes unstable and is transformed into hcp-Ti during heating of as-deposited Ti films.

Table I shows the calculated Mulliken bond overlap populations (OP) between Ti atoms, Ti and H atoms, and Ti and N atoms for the employed models. The values of OP refer to the strength of covalent bonds. The Ti-Ti OP for the Ti_{19} cluster is evaluated to be 0.231. The OP between Ti atoms such as B and C atoms bonding to the nitrogen G atom for the Ti_{19}N cluster in Fig. 5(c) is evaluated to be 0.135, which is much smaller than that for the Ti_{19}, irrespective of the same Ti-Ti bond length. The Ti-N OP (0.277) for the Ti_{19}N is larger than the Ti-Ti OP for the Ti_{19}. The OP between the face-centered A atom and the atoms B, C, D and E in Fig. 3(d) for the Ti_{19}N_{13} cluster is evaluated to be 0.042, which is much smaller than that for the Ti_{19}, while the OP value of Ti-N covalent bonds is 0.289, which is larger than that of Ti-Ti covalent bonds for the Ti_{19}. Comparing the values of OP of Ti_{19}H_8 with those of Ti_{19}H_7, it can be seen that the release of the hydrogen atom denoted by V from the Ti-site leads to the increase in the OP values of such Ti-Ti bonds of tetrahedron without hydrogen as B-C, B-N, N-C bonds, whereas the OP values of such Ti-Ti bonds of tetrahedron with hydrogen as B-S, B-U bonds does not differ so much. Moreover, the OP of Ti-Ti bond such as B-R bond becomes relatively large, accompanying with the release of hydrogen in the tetrahedron such as BCNR in Fig. 5(b). Thus, it can be considered that the strengthening of the B-R bond promotes the shear in the (112) direction on the (111)-plane including B, C, N atoms in Fig. 5(b). This shear direction corresponds to the direction of AC in Fig. 2(b). It is noted that atoms denoted by alphabetical letters in Fig. 5(b) correspond to those in Fig. 2(b) and then to open circles denoted by alphabetical letters with asterisks in Fig. 2(a). Therefore, in order to obtain an hcp lattice by the fcc-hcp transformation, the atoms on the (111)-plane including B, C, N atoms in Fig. 5(b) have to be shifted. The direction of shift is the (112) direction. After the shift, the B atom in Fig. 5(b), for example, has to be at the center of gravity of the BCN triangle. The direction of the shift is on the projected line of line BR to the (111)-plane including B, C, N atoms in Fig. 5(b). This shift of the (111)-plane agrees with the shift of open circles denoted by alphabetical letters with asterisks to solid circles denoted by the same alphabetical letters without asterisks of hcp-Ti in Fig. 2(a). Thus, the shift of the B atom to the center of gravity of the triangle BCN promoted by the forming of the stronger B-R bond for Ti_{19}H_7 than that for Ti_{19}H_8 and the resultant shift of the triangle BCN ((111)-plane) accompanied by the strengthening of the B-C, C-N and N-B bonds in Fig. 5(b) can be considered to be the origin for the fcc-hcp transformation of Ti sublattices.

The value of OP of each bond between Ti atoms for the Ti_{19} and Ti_{19}N cluster models in Fig. 5 has been inspected in detail, and is shown in Table III. Table III shows the exis-

TABLE III: Overlap population of each bond between Ti atoms for the Ti_{19} and Ti_{19}N cluster models shown in Figs. 5(a) and 5(c).

| Cluster Model | A-B, atoms | A-I, atoms | C-B, atoms | C-I, atoms |
|---------------|------------|------------|------------|------------|
| Ti_{19}       | 0.231      | 0.231      | 0.319      | 0.319      |
| Ti_{19}N      | 0.135      | 0.254      | 0.200      | 0.348      |
tence of relatively large differences between the OP value of A-B, A-C, A-D, A-E atoms and that of A-I, A-H atoms, and between the OP value of C-B, D-E atoms and that of C-I, D-H atoms for Ti$_{19}N$, compared with those for Ti$_{19}$. This indicates that bonds between Ti atoms of the octahedron occupied by N atom at the center, as the octahedron ABCDEF in Fig. 5(c), weaken, whereas bonds between Ti atoms of the octahedron not occupied by N atoms, as the octahedron ACDHII, do not change, or rather strengthen a little. The weakening of Ti-Ti bonds caused by the occupation of the O-sites by N atoms promotes expansion of the spacing between (00 • 1)-planes, which results in the TEM-observed lattice expansion in the c-axis of hcp-Ti by N-implantation [14]. On the other hand, the OP of Ti-N bonds as A-G and F-G bonds indicated by dotted lines is 0.277, and becomes relatively large compared with the OP of Ti-Ti bonds in the octahedron ABCDEF for Ti$_{19}N$. Thus, it can be considered that the strengthening of the A-G and F-G bonds promotes the shear in the FL (01 • 0) direction on the (00 • 1)-plane including B, E, F atoms for Ti$_{19}N$. This shear direction corresponds to the direction of BW in Fig. 2(a): in order to obtain an fcc sublattice by the hcp-fcc transformation, the atoms on the (00 • 1)-plane including B, E, F atoms for Ti$_{19}N$ have to be shifted. The direction of shift is the FL (01 • 0) direction. After the shift, the F atom, for example, has to be at the center of gravity of the triangle BEF. The projected line of line FA to the (00 • 1)-plane including B, E, F atoms for Ti$_{19}N$ is on the line FL. The inheritance of square atomic arrangement formed by C, D, H and I atoms during the hcp-fcc transformation, which agrees with the inheritance of square atomic arrangement formed by E, F, J and K atoms in Fig. 2(a), is responsible for the epitaxial growth of TiN$_y$. Thus, the shift of the F atom to the center of gravity of the triangle BEF promoted by the forming of the strong A-G and F-G bonds and the weakening of the C-B and D-E bonds for Ti$_{19}N$ and the inheritance of square atomic arrangement formed by C, D, H and I atoms can be considered to be the origin for the hcp-fcc transformation of Ti sublattices and epitaxial growth of TiN$_y$.

IV. CONCLUSIONS

Both hcp-Ti and CaF$_2$-type TiH$_x$ ($x \approx 1.5$) with preferred orientations have been grown in as-deposited Ti films on NaCl (001) substrates held at RT. The Ti films were heated up to 350°C in the TEM combined with ion accelerators. In order to clarify atomistic growth processes of TiN$_y$ films due to N-implantation into the Ti films, changes of the crystallographic and electronic structures of Ti thin films by heating and by nitriding during N-implantation were investigated by in-situ observations of TEM and EELS, with the aid of DV-Xα calculations. H atoms which constituted TiH$_x$ were released from the as-deposited Ti films with heating, and were completely released at 350°C. The H-released unstable fcc-Ti sublattice was transformed into hcp-Ti. The loss peak by EELS for TiH$_x$ shifted to the lower energy side due to the release of H atoms from TiH$_x$ during heating. The shift of the atoms on the (111)-plane in the (112) direction, promoted by the forming of the stronger Ti-Ti bond due to the release of H atoms can be considered to be the origin for the fcc to hcp transformation of Ti sublattices. On the other hand, the TiN$_y$ is epitaxially formed by the N-implantation into the hcp-Ti films, through the transformation of the hcp-Ti to fcc-Ti sublattice, partially inheriting the atomic arrangement of the hcp-Ti and accompanying the occupation of O-sites by N atoms. The loss peak during N-implantation into hcp-Ti films gradually shifted to the higher energy side with the increase in dose, due to the increase in the electron density in the hybridised valence band. The bonding interaction of Ti sublattices with N atoms gives rise to the forming of stronger covalent bonds, and to the weakening of Ti-Ti bonds. Thus, it is considered that the shear in the (01 • 0) direction of hcp-Ti promoted by the forming of the strong Ti-N bonds and the weakening of the Ti-Ti bonds is the origin for the hcp-fcc transformation of Ti sublattices. Therefore, it is concluded that the shift of the atoms on the closed-packed plane induced by the change of bonding interaction of Ti sublattices with ligand H or N atoms plays a important role in the transformation between fcc-Ti sublattices and hcp-Ti sublattices due to the release of H atoms or due to the occupation by N atoms.

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