the thickness of the wall of 0.7 nm to calculate specific gravity.

The specific gravity of allophane can be obtained from the molecular weight of allophane to the volume of one unit allophane particle. The obtained specific gravity of allophane is used to calculate the volume of the inner sphere of allophane. By assuming that water molecule will fill the inner sphere, the amount of water retained can be calculated according to the specific gravity of H_2O, 1.0 g cm^{-3}. The external diameter was varied from 3.5 to 5.0 nm whereas the thickness of the wall was fixed as 0.7 nm.

Because the structure is ball-shaped and there is space within the wall, the total surface area of allophane covers external and inner surface of the ball, excluding the surface area of the pore regions. The calculated total specific surface area can be obtained from the sum of the external and inner surface areas then subtracted by the surface area of the pore regions. In our calculation, the pore regions of allophane are assumed to be cylindrical with a diameter of 1.0 nm.

CHEMICAL STRUCTURE OF ALLOPHANE

We found that regularity of the polyhedron could be used to build up the basic structure of nano-ball allophane. This polyhedron is composed of eight hexagonal gibbsite sheets with orthosilicic acid bonded to it. This structure has open cage structures of which the wall is hexagonal shape and the pores are tetrahedral shapes. The bond distances of Al-O and Si-O were taken as 0.192 nm and 0.162 nm, respectively, in according with the values in similar minerals, while Al atoms were taken as forming a regular octahedral structure and Si atoms as forming a regular tetrahedral structure. The complete chemical structure of allophane with external diameter of 4.25 nm is presented in Fig. 1. It has molecular weight of 46510 and Si/Al atomic ratio 0.574. It has six holes with diameter about 1.0 nm and lattice parameters of a=b=c= 4.14 nm with a=90.0 degrees.

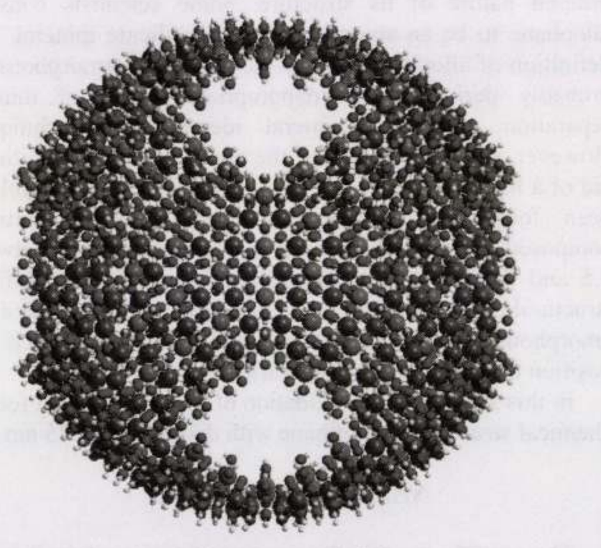

Fig.1 Chemical structure of allophane nano-ball.

The complete chemical structure of nano-ball allophane has the symmetry of Th and the point group is m3. There are two kinds of rotation axes. First, the 3-fold axes (C_3–axes) passing through the center of the hexagonal planes. It takes a rotation of 120 degrees to map the molecule onto itself. Since there are 8 hexagonal planes, there are 8 different 3-fold axes. Second, the 2-fold axes (C_2–axes) pass through the center of the pores. The molecule is symmetric under a rotation of 180 degrees. Likewise, since there are 6 tetrahedron planes, there are 3 different 2-fold axes. There are 8 S_6–axes, in which C_3–axes become S_6–axes, and a center of inversion appears.

The mirror symmetry is related to the edge of the hexagonal planes. There are 3 mirror symmetry planes in this structure. Two vertical planes as C_2–axes passing through the center of the pores and a single horizontal C_2–axes at the intersection of two mirror planes.

SPECIFIC GRAVITY

The density of allophane is between 2.72 to 2.78 g cm^{-3} and the amount of water retained in space within the wall is 0.11 g g^{-3}). By combining with electron microscopic data, Wada and Wada[3] also showed that allophane has a unique arrangement, namely a hollow spherical structure unit, with an external diameter of between 3.7 and 5.5 nm and wall thickness about 0.7 to 1.0 nm.

The calculated specific gravity of the nano-ball allophane model with a diameter of 4.25 nm is 2.75 g cm^{-3}. This result is in good agreement with experimental data determined by the water displacement method[3]. Fig. 2 shows the calculated water retained in the inner sphere. The water retained in the space inside the wall is calculated as 0.16 g g^{-3} with external diameter of 4.25 nm. The volume of inner sphere is close to experimental data regarding the volume of the inner sphere of allophane.

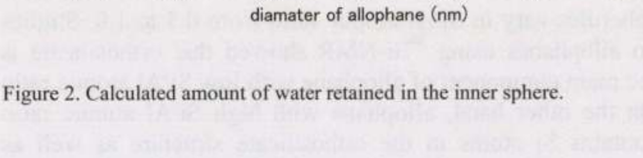

Figure 2. Calculated amount of water retained in the inner sphere.

SPECIFIC SURFACE AREA

Allophane is known to have high specific surface area and high value of the relative micropores, compared with layer silicates such as montmorillonite. The surface area of allophane has been measured to be in the range of 700-900 m^2 g^{-1} by EGME method[4]. On the other hand, the surface area of allophane has a range of about 1200-1365 m^2 g^{-1} measured by the water absorption method[5].

Fig. 3 shows calculated total surface area, external surface area and internal surface area of nano-ball allophane. The calculated total surface area is 1114 m^2 g^{-1} with external