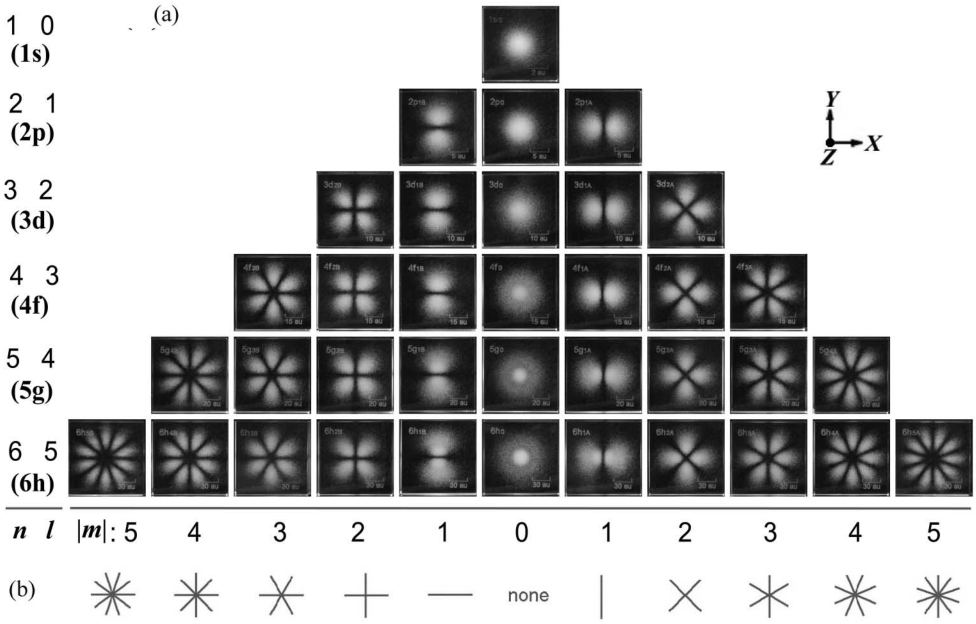

Fig. 8. (a) Probability density distribution in the 3-dimensional representation of the squares of hydrogen atomic orbitals observing through z axis Glass size: $4 \times 4 \times 4$ cm. (b) Schematic representation of the planar nodes containing z axis.

In the case of 2p (y) or 2p (x) orbital, $|m|$ is equal to 1, corresponding to a single horizontal or vertical line in Fig. 8(b) [16].

In Fig. 8(a), the absolute value of magnetic quantum number $|m|$ is the same in every orbital drawn up in a column, giving the same pattern as is shown in Fig. 8(b).

In the case of $m \neq 0$, there exists a pair of orbitals having the same quantum number n, l, and $|m|$. When rotating around z axis by 90 degrees$/|m|$, the planar nodes containing z axis in one part of this pairing orbitals can be transformed to the pattern of corresponding nodes of the other part of the pairing orbitals.

At a glance, the form of atomic orbitals seems to be full of chaos [17], however, by the classification according to the node type in Fig. 7(a) or Fig. 8(a), we can see systematic regularity shown in Fig. 7(b) or Fig. 8(b).

8. Relationship between an Absolute Square of Complex Atomic Orbital and a Real Atomic Orbital

In the case of $m \neq 0$, atomic orbital functions (3) in Fig. 3 are all complex. Isosurfaces of squares of these complex and also $m = 0$ wavefunctions are shown in Fig. 9(a). By taking linear combinations of a pair of complex wavefunctions, the well known real atomic orbitals (4) are obtained [10–12]. Isosurfaces of these real wavefunctions are shown in Fig. 9(b).

Examples to obtain “real function form” by slicing up “absolute square of complex function form” of hydrogen 3d orbitals with $|m|$ planar node(s) are shown in Fig. 10 [17–19].

When $n = 3, l = 2$, and $m = 0$ (Fig. 10(a)), there exists no planar node containing z axis. There is no slicing up, therefore, the shapes of the resultant orbital (bottom) are the same as the top view except for their mathematical signs expressed by their colors.

When $n = 3, l = 2$, and $|m| = 1$, the number of planar nodes containing z axis is 1. The mathematical process to give Eq. (13) can be viewed geometrically as slicing up the two doughnuts with one planar node containing z axis (Fig. 10(b) top, right) and with the edges rounded off to get the clover type 3d (xz) orbital (Fig. 10(b) bottom, right). As for the Eq. (14), slicing the two doughnuts with a node perpendicular to this (Fig. 10(b) top, left), we get the pairing clover type 3d (yz) orbital (Fig. 10(b) bottom, left).

When $n = 3, l = 2$, and $|m| = 2$, the number of planar nodes containing z axis is 2, therefore, two equally spaced planar nodes are used to slice a single doughnut, the familiar clover type four lobes of 3d $(x^2 - y^2)$ orbital is given (Fig. 10(c), right). When the two equally spaced planar nodes are rotated around z axis for 45 degrees and are used to slice a single doughnut, the familiar clover type four lobes of 3d (xy) orbital is given (Fig. 10(c), left).

Figure 9(b) shows the result of slicing the “doughnut-like” lobes into lobes using $|m|$ planar nodes containing z axis. For each non-zero value of $|m|$, a pair of real orbitals are given. These two orbitals have the same shape and by the rotation around the z axis by 90 degrees$/|m|$, one of the pair is transformed into the other pair. In Fig. 9(b), only one of the pair is shown.

A three dimensional representation of the probability density of a complex or real hydrogen atomic orbital in a spherical glass block was developed. Different from a cubic media in Fig. 7(a) or 8(a), a spherical media has no edge. This advantage is effective for the observation of $n = 1, 2, \ldots, l = n - 1, m = 2$ orbitals. In the case of fourth column in Fig. 8(a), planar nodes containing z axis is clearly seen as is shown the one of them in the fourth column in Fig. 7(a). However, as for the pairing orbitals shown in the eighth column in Fig. 8(a), it is difficult to observe planar nodes containing z axis because of the hindrance of