of the oligonucleotide in the presence of a variety of metal ions [2] (Mg^{2+}, Mn^{2+}, Ca^{2+}, Ni^{2+}, Sr^{2+}, Ba^{2+}, Cd^{2+}, Cu^{2+}, $Co(NH_3)_6^{3+}$, Zn^{2+} y Li^{+}) to stabilize the structure of the crystal. By X-ray diffraction we obtained patterns with low resolution from which in a first stage, it was only possible to determine the cell parameters and space group. The best crystals were obtained in presence of cadmium which has a high affinity for adenine bases. Contrary to common behavior of A-T rich oligonucleotides, when hairpin has been stabilized with cadmium the best crystals are obtained at 21°C, while using the other metal ions low temperatures is needed to obtain crystals; usually between 4 and 11°C. On the other hand, by performing DLS analysis was detected the influence of cadmium in the structure stabilization and in the intermolecular contacts stabilization, which compared to the magnesium interaction and the reference without metal ion is higher. Also by DLS analysis we confirmed the formation of the DNA hairpin by monitoring the diffusion coefficient and size of monomeric species. We constructed hairpin and duplex DNA theoretical structures and performed a simulation of the diffraction obtaining a model of molecular packing. We may assume the formation of a DNA hairpin from 100% A-T oligonucleotides and highlight the role of metal ions on the hairpin stabilization.

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Keywords: hairpin, oligonucleotide, crystallization

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Crystal structures of two CBSX proteins from *Arabidopsis thaliana*

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CBS (cystathionine-β-synthase) domain is a small intracellular module, mostly found in two or four copies within a protein, which has been identified in many proteins in all kingdoms of life. Tandem pairs of CBS domains can act as binding domains for adenosine derivatives and may regulate the activity of attached enzymes or other domains. Many proteins containing CBS domain are easily identified in plant genome. However, their exact physiological functions remain elusive. Two of them, AtCBSX1 and AtCBSX2 (CBS pair protein) from Arabidopsis thaliana have been cloned and analyzed. These encode 236 and 238 amino acid residues which contain two tandem CBS domains, respectively. Both proteins were over-expressed heterologously in E. coli and purified them as homogeneity. The structure of AtCBSX1 and AtCBSX2 determined at 2.2 and 1.9 Å resolution, respectively, reveals an unique architecture and a positively-charged pocket for AMP. The structure of AtCBSXs show that it is an anti-parallel dimer on its central two-fold axis and show a uniquely ~120º bent at the side whereas all the other parallel CBS domain proteins are approximately flat ~180º. However, the structure of dimeric AtCBSX2 with bound AMP is show approximately flat, which is significantly different from the apo form of that. This orientation, shape, molecular symmetry of AtCBSX protein and more importantly conformational change induced by ligand-binding might determine the interacting surface for binding molecules, which is related to its function.

Keywords: X-ray, structure, conformational change

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Structural and functional studies of the active-sites in four glycoside hydrolase β-jellyroll families

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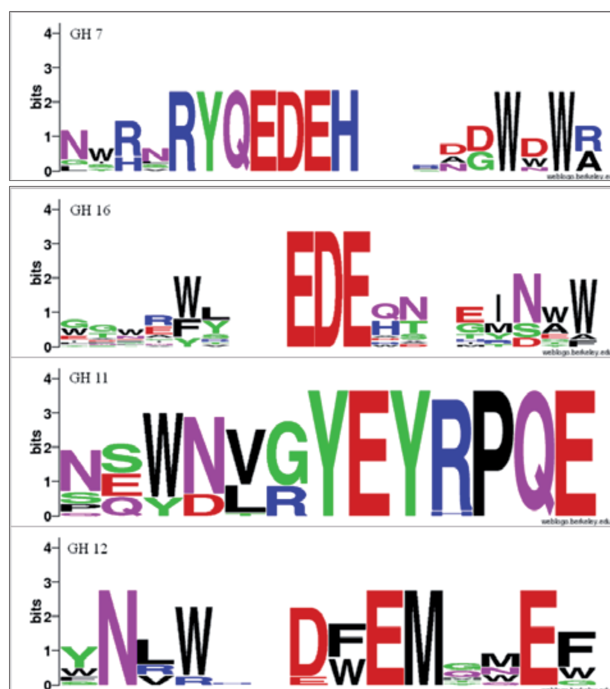
The three-dimensional (3D) structure of glycoside hydrolase family (GHF) 7, 11, 12 and 16 are collectively referred to as a jellyroll β-sandwich fold with a similar cleft catalytic active site, although the amino acid sequences of these four families are diverse. Based on the results of primary sequence alignment and 3D structural comparison, GHF 7 and 16 possess a conserved catalytic motif of RYQExDxEHWW and ExDxE/ExDxxE, whereas GHF11 and 12 share a general active site motif of $YE_nYPQE_{n+(88\sim94)}$ and $NE_nME_{n+(83\sim97)}$, respectively. The first and last glutamyl residues found in the catalytic motifs have been clearly identified as catalytic nucleophile and general acid/base for retention hydrolytic mechanism, respectively. A detailed structural comparison among the known structures reveals that they share a low level of amino acid sequence identity 5~20%, but the enzymes have a high degree of structural conservation at the active sites.



Keywords: glycoside hydrolase β-jellyroll family, conserved amino acid, structural and primary sequence comparison

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Crystal structures of symbiosis related lectin and its saccharide bound form

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Lectins are sugar-binding proteins or glycoproteins that recognize specific carbohydrate structures and agglutinate various types of animal cells. In marine animals, lectins are believed to contribute as non-self recognition factors to the defense mechanism. Interestingly, it has been theorized that some lectins from marine animals mediate the interaction between symbiont and host. SLL-2 is a D-galactose binding lectin isolated from an octocoral, *Sinularia lochmodes*. It was found that SLL-2 was distributed densely on the surface of symbiotic dinoflagellate *Symbiodinium* sp. cells. Previous report showed that SLL-2 transforms free-swimming stage *Symbiodinium* cells into non-motile stage *Symbiodinium* cells and keep them in their non-motile stage [1,2]. These results show that SLL-2 is a chemical cue in the symbiosis between dinoflagellates and coral. The three-dimensional structure of SLL-2 will provide information about the symbiosis mechanism.

The structure of SLL-2 was determined by the molecular replacement method using atomic coordinates of *Helix pomatia* agglutinin (HPA lectin, PDB code: 2ccv) as a search model. Three SLL-2 monomers form a trimer around a non-crystallographic 3-fold axis, and two trimers form a hexameric assembly using hydrogen bonds of three pairs of elongated strands from each monomer. The crystal structure of SLL-2 monomer shows the beta-sandwich lectin fold with six strands. The sites of N-glycosylation and sugar binding (“site 1”) were identified clearly in the monomer structure. In the hexameric molecule, two of the six “site 1”s possess galactopyranoside derivative that might come from the N-glycosylation site, three contain the precipitant molecule, and the remaining one accommodate a water molecule. Crystals from low monosaccharide (GalNAc: N-acetyl-D-Galactosamine) concentration holds three GalNAcs and three precipitant molecules in its “site 1”s. The crystal structure of SLL-2-GalNAc complex from sugar-rich environment indicated that GalNAc molecules bind to all “site 1”s. These observations reveal that SLL-2 can maintain both unsymmetrical and symmetrical hexameric molecule stably across various environments. In addition, a large electron density, which appears for a part of oligosaccharides but was not enough to ensure the bound species and its orientation, was observed at extra sugar binding site, “site 2”. From these results, we could propose binding mode of the pentasaccharide, which is the unbranched polysaccharide recognized by HPA lectin, to SLL-2, and the function of the SLL-2 in the symbiosis between dinoflagellates and coral.

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Keywords: lectin, coral, symbiosis

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Interface Plasmon in Pseudo One-dimensional Si/SiO_2 core-shell Nanostructures by Electron Energy Loss Spectroscopy

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Surface/interface plasmons (IP) in nanostructured materials has generated much interest for their potential applications in plasmonic devices, in particular, those can be operated beyond the diffraction limit of light. While the plasmonic properties of nanomaterials are commonly studied using optical approaches, the best spatial resolution achieved is a fraction of optical wavelength, i.e., ~50 nm. Consequently, mapping of plasmonic properties at higher spatial resolution and imaging of nanostructures of smaller than about 50 nm remains difficult. On the other hand, TEM-EELS has been recently employed as alternative technique for such purposes [1]. The excellent spatial resolution of the technique enables the mapping of local variations in the material’s dielectric response at nanometer scale. Although caution has to be taken, qualitative agreement between the EELS results and material’s photonic response make it a powerful tool in probing the local plasmonic properties of nano-objects. Furthermore, the TEM allows to obtain chemical and structural information from the *same* area as the plasmon maps.

The interface plasmon in pseudo one-dimensional Si/SiO_2 core-shell nanostructures have been investigated using electron energy loss spectroscopy (EELS)-related techniques under parallel illuminations, which results are comparable to those obtained by optical methods.

Elongation from a perfect spheroid Si/SiO_2 core-shell nanoparticle to nanorod, and eventually to a long nanowire, results in splitting of the IP modes to a transverse and a longitudinal branch. The longitudinal IP mode red shifts with the aspect ratio increase of the nanoparticle, due to the larger charge separation distance along the long axis of the nanostructure. Retardation effect comes into play in longer nanostructures, leading to periodical pile up of opposite charges. This is revealed by the uniform intensity along the longitudinal direction of the long Si/SiO_2 nanocable in the energy filtered image. The small diameter of the nanostructure determines the dominance of the longitudinal mode in the IP oscillation. Consequently, the optical absorption of small-diameter nanostructures is significantly different from that of the larger ones.

Assembly of the Si nanoparticles into one-dimensional particle chains leads to interaction between the adjacent nanoparticles, which can also induce the splitting of the interface plasmon into transverse and longitudinal polarizations. In addition, such coupling causes spatial re-distribution of the IP intensity, leading to local field enhancement in-between the two nanoparticles. By controlling the growth of Si nanostructures into different morphologies, we demonstrate that the material’s optical properties can be manipulated.

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Keywords: EELS, plasmon, silicon

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Radiation damage and electron energy loss spectroscopy of Au particles on amorphous Ge substrates

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Ideally the morphology, structure, and electronic properties from an individual nanoparticle would be obtained in a (scanning) transmission electron microscope (S)TEM experiment at an irradiation dose that does not lead to appreciable sample damage. Gold nanoparticles are of interest as catalysts and as building blocks of plasmonics devices. Irradiation of Au particles by an electron beam results in both hopping of individual Au atoms, observed in extremely small clusters, and in frequent change of orientation of particle with respect to the incident electron beam, observed even in particles with volume more than $(10)^3$ nm^3 [1].

A TEM/STEM equipped with a cold field electron source and an electron energy loss (EEL) spectrometer can be used to obtain all the