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Self-similar patterning of inversion domains in Al-Cu-Co decagonal quasicrystals

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We find a striking distribution of inversion domains in a decagonal $Al_{64}Cu_{22}Co_{14}$, which reveals a fractal-like, self-similar microstructure constructed by golden triangles (similar to a Sierpinski Gasket). This unique morphology of domains is confirmed to be thermodynamically stable configurations at high temperatures (> ~1200K), just below the melting temperature of the $Al_{64}Cu_{22}Co_{14}$ compound. Details of the domain microstructure are described based on dark-field TEM imaging, convergent electron diffraction and atomic-resolution STEM. We propose that the occurrence of such self-similar domains may well be understood by concerning structural modulations extended into a hyperspace.

Keywords: quasicrystals, electron diffraction, electron microscopy

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Thermal stability study and structural of palladium platinum nanoparticles by HREM

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Platinum (Pt) Palladium (Pd) nanoparticles supported on amorphous silica (SiO_2) were prepared by wetness impregnation techniques at same concentrations of Pt(0.5) and Pd(0.5); 1 metallic wt %. The particle size distribution were measured as function of reaction temperature, temperatures were varied in the range of 200 ℃ - 400 ℃ to evaluate the nucleation phenomena and thermal stability. In addition morphology and crystallinity under various reactor temperatures were investigated by physisorption Brunauer-Emmett-Teller-(BET), X-Ray Diffraction (XRD), High Resolution Electron Microscopy (HREM) and Transmission Electron Microscopy (TEM). In this work, we observed the distribution of Pt and Pd in nanoparticles. The rational design of nanoscale structures for applications in technology increasingly relies on developing and improved understanding of processes, particularly in terms of how they contribute to the changing phase behavior of nanoscale systems. Crystal structures can be determined by X-ray, while transmission electron microscopy (TEM) is indispensable for characterization of nanocrystalline materials, because TEM is a tool that provides not only atomic resolution lattice images but also chemical information at a spatial resolution, allowing direct identification the chemistry of a single nanoparticle.

Keywords: nanoparticles, metals, HREM

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Morphological studies on single crystals and nanofibers of poly(heptamethylene terephthalate)

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Poly(heptamethylene terephthalate) (PHepT), which is one of aromatic polyesters, was synthesized, and its lamellar single-crystals were grown isothermally, for example at 70℃, from a dilute solution in 1-octanol. Nanofibers of PHepT were prepared *via* electro-spinning (apparatus: esprayer ES-1000 (Fuence Co., Ltd.; Tokyo, Japan)) of a solution in 1,1,1,3,3,3-hexafluoro-2-propanol. Morphology of the single crystals and that of as-spun and annealed nanofibers were investigated with a transmission electron microscope (JEOL JEM-200CS) which was operated at 200kV. Selected-area electron diffraction (SAED) of the crystals gives a well-defined N-pattern consisting of spot-like *hk*0 reflections, and that of a bandle of the annealed nanofibers gives a highly oriented fiber pattern. From the analysis of SAED patterns for both types of specimen, namely single crystals and nanofibers, it seems that PHepT takes an orthorhombic crystal system and its unit cell parameters are as follows: a = 1.409nm, b = 1.480nm, c (chain axis) = 3.392nm, $\alpha=\beta=\gamma=90^\circ$. In addition, dark-field images of the PHepT nanofibers which had been annealed at 85℃ for 2 days were taken by using some of the reflections on/near the equator. The images showed a stacked-lamellar structure, in which crystalline lamellae are stacked in the direction of the fiber axis, and the corresponding average long period was estimated at about 19nm.

Keywords: polymer single crystal, nanofiber, poly(heptamethylene terephthalate)

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EM Navigator - 3D electron microscopy data navigator

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EM Navigator (URL: http://emnavi.protein.osaka-u.ac.jp/) is our new web service for browsing the 3D electron microscopy (EM) structure data, based on the data form EM Databank (EMDB) and Protein Data Bank. It has been constructed so that even users who do not know well about 3D EM can see easily and pleasingly browse the 3D EM data. EM structure data have not been friendly. It is often very hard to recognize the 3D structures just by seeing the figures on the papers or the web pages. In case of atomic coordinates of proteins, we can easily get the 3D views using jV on the PDBj web site or opening the downloaded data using some famous software such as RasMol. On the other hand, it requires some skill and effort to make 3D views like the figures on the papers from data such as 3D maps deposited on the EMDB. The barriers are much higher to view the structure combined with the other data such as the atomic coordinates fitted into the EM map. We have been constructing movies for each the data entry in the EMDB, and embedding them on the EM Navigator web pages. You will get easily the 3D views with the detail information by the

web browsers without installing special software. Further movies will be added, such as the views with the fitted atomic models and the zoomed up views around the important regions. Moreover, we are making the site useful by putting the snapshots of the PDB data published along with the EM data, the images of the supplementary information deposited by authors, and so on.

Keywords: electron microscopy, database, structure

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Structural insight into the mechanism of activation of the Toll receptor

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The Drosophila Toll receptor, which functions in both embryonic patterning and innate immunity to fungi and Gram-positive bacteria, is activated by a dimeric cytokine ligand, Spätzle (Spz). Previous studies have suggested that Spz crosslinks two Toll receptor molecules to form an activated complex. Here we report electron microscopy structures of the Toll ectodomain in absence and in presence of Spz. Contrary to expectations, Spz does not directly crosslink two Toll ectodomains. Instead Spz binding at the N-terminal end of Toll predominantly induces the formation of a 2:2 complex, with two sites of interaction between the ectodomain chains, one located near to the N-terminus of the solenoid, the other between the C-terminal juxtamembrane sequences. Moreover Toll undergoes a ligand-induced conformational change, becoming more tightly curved than in the apo form. The unexpected 2:2 complex was confirmed by mass spectrometry under native conditions. These results suggest that activation of Toll is an allosteric mechanism induced by an end-on binding mode of the ligand.

Keywords: Toll receptor, electron microscopy structures, ligand binding

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Structures of the laminin-binding integrins

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Integrins are a family of cell adhesion receptors that mediate cell-cell and cell-extracellular matrix interactions and govern migration and anchorage of almost all kinds of cells. Mammalian genomes contain 18 alpha and 8 beta subunits that combine to form 24 different hetrodimers, each of which has an apparently unique ligand-binding profile and biological function. Only one atomic structure of integrin alpha(V)beta(3) of full length extracellular domains of 24 dimers has been determined to date. The atomic structure of the integrin alpha(V)beta(3) together with the subsequent structural analysis using electron microscopy revealed that global conformational rearrangements, bent and extended conformations, in integrin extracellular domains regulate the ligand-binding affinity. The conformational change between bent and extended structures suggested a “switchblade” (or jack-knife) model for affinity switching. Furthermore, similar conformational changes were observed in leukocyte beta(2) integrins, alpha(X)beta(2) and alpha(L) beta(2). However, 24 kinds of integrin heterodimers exhibit their own unique ligand-binding activities and function. Unlike the integrins existing in platelets or blood corpuscles including alpha(IIb)beta(3), alpha(V)beta(3), alpha(X)beta(2), alpha(L)beta(2) and so on, integrin alpha(3)beta(1), alpha(6)beta(1), alpha(7)beta(1) and alpha(6) beta(4) constantly bind to their ligands, laminins at the basement membrane. Therefore, we focused on the laminin-binding integrins and determined the structures by the electron microscopy to address the ligand specific integrin-ligand binding mechanism.

Keywords: electron microscopy, cell adhesion, structural biological function

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Electrostatic potential analysis of the ferroelectric phases of perovskite oxides using CBED

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We have been developing a method to refine crystal structural parameters using convergent-beam electron diffraction (CBED), which can determine atom positions, Debye-Waller factors (atomic displacement parameters) and low-order structure factors from a nanometer-size area of specimens. The electrostatic potential and electron density distributions are reconstructed from the refined parameters. Especially for the determination of electrostatic potential, CBED is more advantageous than the X-ray method because the Fourier coefficients of electrostatic potential are directly determined and the electrostatic potential is reconstructed without any errors caused by the conversion of structure factors. The electrostatic potential consists of the positive contribution from nuclear charge and the negative one from electrons. The behaviors of valence electrons alter the balance between the contributions of nuclear charge and electrons, which may cause large changes in the electrostatic potential. We have applied the method to the ferroelectric phases of perovskite oxides such as $BaTiO_3$ and $PbTiO_3$. Energy-filtered CBED patterns were obtained from a single domain regardless of the existence of complicated ferroelectric domains. The direction of ferroelectric polarization can be readily identified from the CBED patterns due to the strong dynamical diffraction effect. Electronic polarizations of the atoms have been observed through electrostatic potential gradients, which are caused by relative shifts between the nuclear charge and electrons.
References: [1] Tsuda K. & Tanaka M., Acta Cryst. A55, 939 (1999). [2] Tsuda K. et al., Acta Cryst. A58, 514 (2002). [3] Ogata Y. et al., Acta Cryst. A60, 525 (2004).

Keywords: electrostatic potential, convergent-beam electron diffraction, ferroelectrics

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Differential diffraction

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