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

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Differential diffraction

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A new method of processing and analysing electron diffraction patterns is presented that may have numerous analogues in other areas. It is demonstrated here in quantitative convergent beam electron diffraction (QCBED), for very precise measurements of structure factors. The technique maximises the sensitivity of structure factor measurement from diffraction data by almost completely eliminating the diffuse background contributed by inelastic scattering processes, most notably, thermal diffuse scattering (TDS). This is demonstrated in fig. 1. The present work is an extension to [1] and covers both energy-filtered and unfiltered CBED.

[1] P.N.H. Nakashima, Phys. Rev. Lett. 99 (2007), 125506.

[2] Thanks to A. Prof. J. Etheridge, Prof. A. Moodie, A. Prof. A. Johnson, Dr. V. Streltsov, the Australian Research Council (DP0346828) and the Australian and Victorian Partnerships for Advanced Computing.

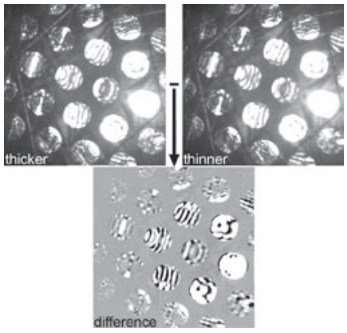

Fig. 1: Two zero-loss-filtered CBED patterns (6eV slit width) from different thicknesses of corundum. The background (outside the discs) in both patterns still contains significant signal due to inelastic scattering (mostly TDS), which is almost completely canceled in the difference pattern.

Keywords: inelastic scattering, thermal diffuse scattering, accurate structure factors

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Automatic space group determination using precession electron diffraction patterns

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A set of algorithms for automatic High Order Laue Zone (HOLZ) indexing and possible set of space groups extraction were developed and implemented in the "Space Group Determinator" program. The symmetry analysis is performed using Morniroli-Steeds tables [1,2]. The developed program becomes extremely useful for the analysis of precession electron diffraction patterns (PEDs) [3]. "Space Group Determinator" was successfully tested on both simulated and experimental diffraction patterns with different zone axis orientations [4]. There are several advantages using PEDs: - The intensities extracted from PEDs are less dynamical, especially for main zone axes; - There are more reflections with higher resolution visible (depending on the precession angle); - The width of a HOLZ band (if visible) can be significantly larger than on a corresponding SAED pattern. The last statement is especially important for the correct space group or set of space groups determination. The possibility to observe several reflection lines within HOLZ makes the plane lattice shifts extraction easier. The knowledge of FOLZ shift with respect to the ZOLZ and the possible differences in periodicities provides very important information. The corresponding plane shifts in a* and b* directions between ZOLZ and HOLZ can be used together with tables from [1] for finding lattice centering, glide planes and partial symmetry symbol. This information can be treated systematically and implemented in the automatic procedure.

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Keywords: space groups, electron diffraction, precession

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Determination of order parameter of single $L1_0$-FePd nanoparticle by nanobeam electron diffraction

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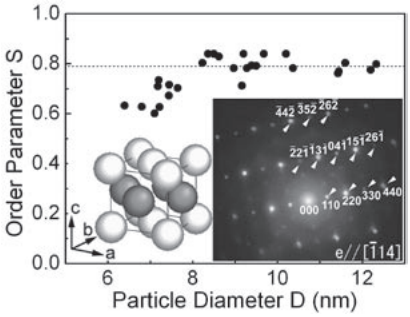
Long-range order (LRO) is the key issue in the structure-property relationships of the hard magnetic FePd nanoparticles with the $L1_0$ structure. In this study, we introduced a new technique to determine the LRO parameter of single FePd nanoparticle using nanobeam electron diffraction (NBD). The LRO parameter was determined by quantitative analysis of NBD intensities recorded by imaging plates together with intensity calculations considering the multiple scattering of electrons. In taking NBD patterns, hh0 systematic reflections were excited using a JEOL 3000F transmission electron microscope. Specimen thickness was evaluated by electron holography. The obtained LRO parameters of nanoparticles larger than 8 nm are distributed around the average LRO parameter (S=0.79) determined by selected area diffraction. In contrast, the LRO parameters gradually decrease as the particle size decreases below 8 nm (S=0.60-0.73). Experimental conditions required for NBD analysis are presented and the possible experimental errors are discussed. Attached figure shows the size dependence of the LRO parameters. A schematic of the $L1_0$ structure and an example of NBD pattern are shown in the inset.



Keywords: microdiffraction, ordered structures, nanoparticles

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Contrast reversal of unindexed Kikuchi lines

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Kikuchi patterns can contain the unindexed line which runs along the middle line of a Kikuchi band and cannot be indexed as a Kikuchi lines. It appears as an excess, deficient or excess-deficient line