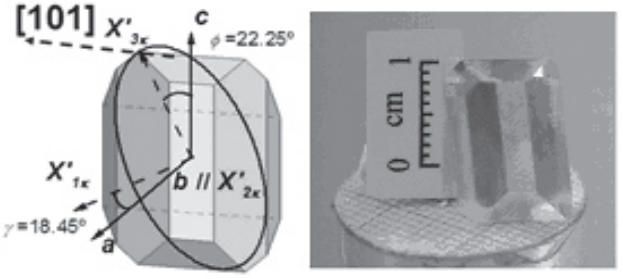
which are N_g, N_m and N_p. N_p corresponds to the ***b*** crystallographic directions, and N_g and N_m are located in the (010) plane; N_g is located 18.5º clockwise from c crystallographic direction.

Such a thermal anisotropy in the monoclinic double tungstates leads to thermal lensing at high power operating levels. Focusing of the light in the crystal provokes high intensities so that the temperature increases significantly producing a mechanical deformation of the crystal, which in consequence, leads to a self-lensing material.

The laser experiments for power scaling carried out with Yb:KLuW in the thin disk configuration at high pump powers reached 9 W in cw regime showing a significant improvement in the thermal management due to the one-dimensional heat flow. This could be known thanks to the deep knowledge on the thermal properties of the monoclinic double tungstate crystals.



Keywords: thermal anisotropy, double tungstate crystals, high power lasers

MS.28.5

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The optical spectra of $Sr_2SiO_4:Eu^{2+}$ nanocrystals

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Sr_2SiO_4 has two polymorphs: β-Sr_2SiO_4 (monoclinic) and α'-Sr_2SiO_4 (orthorhombic). There are two Sr^{2+} sites of ten-coordinated Sr(I) and nine-coordinated Sr(II) by oxygen atoms, which result in two emission bands at around 490 nm and 560 nm by doping Eu^{2+} ions. The various synthesizing methods such as a solid-state reaction and chemical preparations have been widely reported.

In this work, $Sr_2SiO_4:Eu^{2+}$ nanocrystals were prepared by a co-precipitation method using metal nitrates and 3-aminopropyltriethoxysilane (APTES) as a silicon source. NH_4Cl was used as a flux. The as-prepared powders were annealed with different temperatures under H_2 atmosphere in an electric tube furnace. The particle size and morphology were observed by a field-emission scanning electron microscope. X-ray diffractometer (XRD) and photoluminescence (PL) system were used to determine the crystal structure and the photoluminescence spectra, respectively. The effects of the preparation parameters on the structure of the nanocrystals and luminescent properties were investigated. With increasing the annealing temperature the crystallinity was enhanced, showing thin nanorod with the high aspect ratio. The PL spectra exhibited two emission bands at around 485 and 540 nm, indicating that Eu^{2+} ions were successfully substituted for two cation sites of Sr(I) and Sr(II). The preference of Eu^{2+} ions for Sr(I) or Sr(II) strongly depended on the preparing parameters such as the amount of a flux, firing temperature/time, and the Eu^{2+} concentration.

Keywords: luminescence, strontium, silicate

MS.29.1

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Perspectives on the crystal structure of human adenovirus

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Replication-defective and conditionally replicating adenovirus (AdV) vectors are currently being utilized in ~25% of human gene transfer clinical trials. Rational development of adenovirus vectors for therapeutic gene transfer is hampered by the lack of accurate structural information. The recently determined X-ray structure of an adenovirus vector at 3.5 Å resolution of the 150-MDa virion containing nearly 1 million amino acids represents a milestone as the biggest bio-molecular structure yet determined using X-ray diffraction methods (Reddy et al., 2010). The crystal structure revealed interactions between the major capsid protein (hexon) and characteristic structural elements of several accessory molecules that stabilize the AdV capsid. Interestingly, the virus structure also showed an altered association, a symmetry mismatch, between the 5-fold symmetric penton-base proteins and the 3-fold symmetric fiber proteins, where the trimeric shaft of the fiber proteins was seen buried deep inside pore formed by the penton base subunits at the particle vertices. The near atomic resolution structure highlights significant advances in understanding the stabilizing interactions, virus assembly and cell entry mechanisms of a large dsDNA virus and provides new opportunities for improving adenovirus-mediated gene transfer.

V.S. Reddy, S.K. Natchiar, P.L. Stewart, G.R. Nemerow *Science* **2010**, *329(5995),* 1071-5.

Keywords: adenovirus, capsid, structure

MS.29.2

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Structures of porcine adenovirus type 4 and bacteriophage T4 long tail fibres

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Certain viruses and bacteriophages use fibre proteins to bind to their host receptors. Examples are adenovirus, reovirus, and the T-even bacteriophages. These trimeric fibres have been shown to contain novel triple-stranded beta-structures. Here we present structures of porcine adenovirus type 4 fibre and of the tip of the bacteriophage T4 long tail fibre.

Adenovirus isolate NADC-1, a strain of porcine adenovirus type 4, has a fibre containing an N-terminal virus attachment region, shaft and head domains, and a C-terminal galectin domain connected to the head by an RGD-containing sequence. The crystal structure of the head domain is similar to previously solved adenovirus fibre head domains, but specific residues for binding the coxsackievirus and adenovirus receptor (CAR), CD46, or sialic acid are not conserved. The structure of the galectin domain reveals an interaction interface between its two

carbohydrate recognition domains, locating both sugar binding sites face to face. Sequence evidence suggests other tandem-repeat galectins have the same arrangement. We show that the galectin domain binds carbohydrates containing lactose and N-acetyl-lactosamine units, and we present structures of the galectin domain with lactose, N-acetyl-lactosamine, 3-aminopropyl-lacto-N-neotetraose, and 2-aminoethyl-tri(N-acetyl-lactosamine), confirming the domain as a bona fide galectin domain.

Bacteriophages are the most numerous organisms in the biosphere. In spite of their biological significance and the spectrum of potential applications, little high-resolution structural detail is available on their receptor-binding fibres. We present the crystal structure of the receptor-binding tip of the bacteriophage T4 long tail fibre, which is highly homologous to the tip of the bacteriophage lambda side tail fibres. This structure reveals an unusual elongated six-stranded anti-parallel beta-strand needle domain containing seven iron ions coordinated by histidine residues arranged co-linearly along the core of the biological unit. At the end of the tip, the three chains intertwine forming a broader head domain, which contains the putative receptor interaction site. The structure reveals a previously unknown beta-structured fibrous fold, provides insights into the remarkable stability of the fibre, and suggests a framework for mutations to expand or modulate receptor-binding specificity.

Keywords: host cell attachment, beta-structure, tandem-repeat galectin

MS.29.3

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The cell fusion proteins of the "FF" family are homologous to class II viral fusion proteins

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Structural studies of viral membrane fusion proteins have provided key information to understand the process of virus-cell membrane fusion, which is important during virus entry. Similar principles were inferred from structural studies of SNARE proteins, responsible for fusion of intracellular vesicles with their target membranes within the cell. No data are currently available on cellular fusion proteins responsible for cell-cell fusion, a process that is of high relevance during developmental biology and organogenesis.

We report here the crystal structure of a cell fusion protein from the nematode *C. elegans*, termed "Eff-1", where it plays a key role during organogenesis. This protein is the prototype of the "Fusion Family" (FF) of proteins recently described. The structure provides unanticipated evolutionary links with the class II viral fusion proteins observed in regular enveloped viruses. Eff-1 folds as three beta-sheet-rich domains, assembled as a trimer organized as in the post-fusion structures of the alphaviruses and flaviviruses envelope proteins. This type of fusion proteins had so far been observed only in regular envelope viruses, where they make an icosahedral coat completely enclosing the viral membrane in their pre-fusion form. This presentation will describe the structure and provide a model for its putative mechanism of action.

Keywords: cell-cell fusion, developmental biology, structural biology, class II viral fusion proteins

MS.29.4

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Structural basis for the inhibition of apoptosis by Epstein-Barr virus BHRF1

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Viruses must evade host apoptotic defences to ensure their own survival. Despite the complexity of mammalian cell death processes, viruses have evolved successful mechanisms for subverting the apoptotic machinery, including homologs of the mammalian pro-survival protein Bcl-2. The ubiquitous Epstein-Barr virus (EBV), a member of the gamma-herpesviruses, infects the epithelium of the oropharynx and resting B cells. Acute infection manifests as infectious mononucleosis or glandular fever, whereas chronic EBV-associated transformation is associated with Burkitt's lymphoma, Hodgkin's disease and nasopharyngeal carcinoma. EBV BHRF1 is a sequence, structural and functional homologue of Bcl-2, however its mechanism of action remained unclear. Previous structural studies indicated that BHRF1 lacks an accessible BH3 binding groove, and shows only weak affinity for BH3 ligands. We show that BHRF1 is a potent inhibitor of apoptosis, and confers chemoresistance in mouse lymphoma models similar to mammalian Bcl-2. Next, we determined the crystal structures of BHRF1 in complex with Bim and Bak BH3 peptides and show that in contrast to previous predictions, BHRF1 interacts with these proteins in a manner similar to its mammalian counterparts. Structure-based mutagenesis enabled us to address the molecular mechanisms underlying BHRF1 activity. We demonstrate that BHRF1 can prevent Bak activation by direct interaction, but prevents Bax activation indirectly by sequestering the BH3-only proteins Bim, Puma and tBid. Unlike mammalian pro-survival proteins, BHRF1 does not interact with the selective/sensitizer BH3-only proteins. These studies indicate that BHRF1 might be targeted by small molecule mimetics of BH3-only proteins.

[1] M. Kvansakul, A.H. Wei, J.I. Fletcher, S.N. Willis, A.W. Roberts, D.C. Huang, P.M. Colman, *PLoS Pathogens* **2010,** *6(12):*e1001236.

Keywords: viral, cancer

MS.29.5

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Crystal structure of the N-terminal domain of HIV-1 capsid in complex with an assembly- inhibiting nanobody

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HIV-1 maturation from a non-infectious into an infectious agent is accompanied by morphological changes in its capsid shell, which undergoes a protease-mediated conversion from a spherical into a conical shape; therefore capsid assembly is a target for development of antiviral drugs. Here we report the crystal structure at 2.0 Å resolution of the N-terminal domain of HIV-1 capsid in complex with a nanobody capable of inhibiting mature and immature particles in vitro.