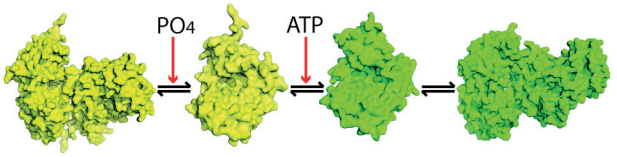
interactions for Rio1 in the presence of adenosine, toyocamycin and ATP revealed interactions between monomers that suggest Rio1 can have two dimeric forms, one observed in the presence of adenosine, and the other seen when bound to ATP and toyocamycin. In addition, since these are both asymmetric, open, dimeric forms, these states have the potential to bind other monomers or dimers to form trimers or tetramers. The dimer formed in the presence of toyocamycin and ATP results in complete occlusion of one active site, consistent with the observation of inhibition by toyocamycin and high concentrations of ATP. Thus, we show that Rio1 activity is influenced by oligomer formation, which is modulated by autophosphorylation and binding to ATP and toyocamycin.



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Keywords: kinase, ribosome biogenesis, oligomer

MS.52.1

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Molecular confinement inside carbon nanostructures: a playground for molecular dynamics investigations

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In this contribution I will present several recent results on the dynamics of a selection of molecules confined inside different nanocarbon hosts: fullerene C_{60} and carbon nanotubes. The results are essentially derived from a large panel of inelastic neutron scattering investigations at different time/energy scales.

In the first part, I will illustrate the effect of confining a quantum system by presenting the results obtained on molecular H_2 confined inside C_{60}[1,2] cages. I'll show how the energy diagram of a free H_2 molecule is affected by the coupling of its translational and rotational degrees of freedom under confinement.

In a second part I will come back to classical physics and will focus on the effect of interstitial insertion of a cubic like molecule C_8H_8 (further referred as "cubane") on the dynamic of the C_{60} lattice. We will see that the cubane molecules act as molecular spacers, resulting in lubrication of the fullerene rotations[3].

In the third part, I will focus on the dynamics of fullerene molecules being the guest molecules when confined onto a 1D lattice inside single walled carbon nanotubes[4], a guest-host molecular system referred as "carbon peapods". The specific spectral signature of the dynamics will be discussed in term of both confinement and low dimensionality.

Keywords: fullerene, neutron_scattering, vibrational

MS.52.2

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Atomic structure of graphitic materials visualized by using TEM and STEM

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Edge structures and atomic defects can significantly affect the physical and chemical properties of low-dimensional materials, such as nanoribbons, and therefore, merit a thorough investigation at the atomic scale. In this study, edge structures of thermally treated graphite have been studied by means of atomically resolved high-resolution transmission electron microscopy (HRTEM). The method for determination of monolayer or more than one layer graphene sheets is established. A series of tilting experiment proves that the zigzag and armchair edges are mostly "closed" between adjacent graphene layers [1]. Besides graphene sheets, the edge structure of monolayered WS_2 nanoribbon has also been investigated by time-resolved annular dark-field imaging (ADF) (as shown in the figure) and spatially resolved electron energy-loss spectroscopy (EELS) with a scanning transmission electron microscope (STEM). Atomic defects, such as vacancies and edge atoms, were unambiguously identified and successfully visualised in motion. We also report a direct observation of slip deformation in the WS_2 nanoribbons and present evidence demonstrating that the deformation process involves the migration of vacancies and rearrangement of W atoms. Single-atom defects were successfully observed for the first time during plastic deformation [2].

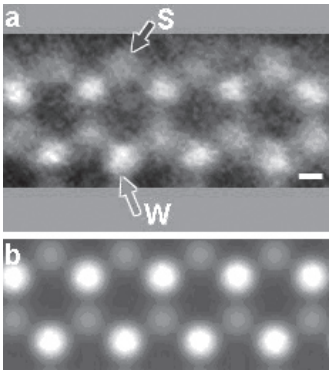

Figure (a) STEM ADF image of a monolayered WS_2 nanoribbon encapsulated inside a SWNT taken in the [001] direction. Scale bar = 0.1nm. (b) The corresponding simulated image.

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Keywords: atomic structure, HRTEM, STEM

MS.52.3

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The physics of nano-carbons explored by high-resolution transmission electron microscopy

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Graphene is a crystalline single layer of carbon atoms that can be described as an individual atomic plane extracted from graphite. It is an outstanding new material that promises a wide range of new

applications and scientific insights [1]. It is also closely related to carbon nanotubes, fullerenes or graphite, which can be described as rolled-up or stacked graphene sheets [2]. Hence, the graphene structure and its defects are of outstanding interest for the science and applications of all these new materials. Static deformations, topological defects, various vacancy configurations or the two-dimensional equivalent of dislocations can be studied by aberration-corrected transmission electron microscopy (TEM) [2-5]. Existing defects in as-synthesized graphene, CVD synthesized graphene, and reduced graphene oxide are analyzed [6-7]. The formation and evolution of defects under electron irradiation is observed in real time with atomic resolution. High-energy electron irradiation provides a "randomization" of some atoms, which then allows new insights into the complicated bonding behaviour in carbon materials [5]. Further, we show that the charge distribution in graphene defects or other 2-D materials can be analyzed on the basis of high-resolution TEM images [8]. I will also discuss important aspects of radiation damage and instrumental performance in the context of radiation sensitive nano-carbon materials.

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Keywords: HREM, graphite, nanotechnology

MS.52.4

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Carbon polyamorphs in pressure-crushed C60 analyzed by scattering tomography

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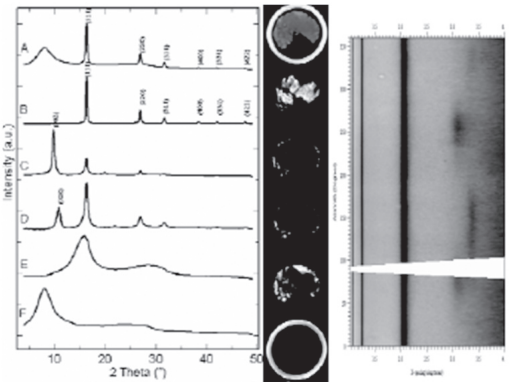
Laboratory carbon samples can be heterogeneous. Among them, the high-pressure polymorphs of C60 are of particular interest for the study of their complex phase diagram and structural properties. We have used scattering resolved tomography (or XRD-CT) as a non-destructive local probe, with depth resolution and structural selectivity [1], to investigate this multi-phased carbon system.

Under hydrostatic pressures C60 molecules are stable up to 20 GPa, but at higher non-hydrostatic compression at room temperature they collapse into polycrystalline cubic diamond and insulating sp3 amorphous phase. Quasi-hydrostatic loading at high temperature produce a conductive graphitic amorphous sp2 structure. Furthermore, HP-HT experiments on C60 allow synthesis of several polymeric and disordered allotropes with a wide range of physical properties [2].

Scattering resolved tomography uses micro-focused synchrotron radiation, allows to extract the spatial distribution of four carbon phases in this system and to recover selectively their scattering diagram (Fig. BCDE). First tomography image corresponds to a full phase reconstruction (all Bragg peaks of the phase were taken into account for the reconstruction). Using selective scattering signal, this probe reveals concentric spatial distribution of cubic diamond, sp3-amorphous diamond, sp2 graphite-like carbon phase and a new ill-ordered carbon phase having an unexpected short interlayer distance of 3.11 Å (Fig. D + unrolled pattern) [3].



Usually in "sp2-graphitic" phases, interlayer distance is found larger than 3.34Å, however it should be noted that in shocked meteorites it was reported a compressed "graphite-like phase" with an 3.19Å interlayer distance and a similar spatial concentric relationship between different carbon polymorphs [4]. Additionally, lattice d-spacing maps on the low compressible diamond phase reveal different strained diamond crystallites in the core of the sample.

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Keywords: diamond, graphite, diffraction-tomography

MS.52.5

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In-situ characterization of the carbon nanotube growth process by X-ray diffraction

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In the last few years carbon nanotubes (CNT) attract more and more attention due to their interesting physical properties especially in the field of micro electronics. Synthesis of CNTs with tailored properties is still a critical point, especially for their applications as interconnects. The growth of CNT by chemical vapor deposition (CVD) is an established synthesis route and it was used in this study.

In-situ X-ray diffraction experiments during growth conditions are performed at the beamline BM20 at the ESRF operated by the Helmholtz-Zentrum Dresden-Rossendorf using a high temperature annealing chamber suitable for reactive gases. Acetylene was used as carbon precursor for the CVD of CNT. Different catalyst systems were studied. For iron nano-particles acting as CNT catalyst, there is still a debate which species can be catalytically active: metallic iron and/or iron carbide. The formation of the metal nano-particles by dewetting and respective crystallisation of the initial thin film was followed by X-Ray reflectivity (XRR) and diffraction (XRD) measurements. We proved that CNT growth can occur without the presence of Fe_3C. In general two reaction pathways denoted by a high and low (or zero) iron carbide concentration were observed. Which route the growth follows depends in a statistical way on the ratio of different iron phases (α - and γ -Fe) present in the nano-particles. This can be influenced also by the reaction conditions like temperature and kind of the buffer