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Solid-state amorphization transitions, induced via heating or the application of pressure, significantly increase the range of materials that might yield amorphous phases. The debate about the materials that result from such transitions is whether they are 'typical' (i.e. similar to those produced via melt-quenching), whether they form a new amorphous class or indeed whether they should be classed as amorphous at all.

Determination of their structure is the key to resolving this debate. Here we use atomistic modelling, based on the reverse Monte Carlo method, of x-ray and neutron diffraction to investigate the structures that result from pressure-induced amorphization (PIA) and temperature-induced amorphization (TIA) of ZrW_2O_8 and the zeolitic imidazolate framework material ZIF-4, respectively. In both cases the amorphous phase forms from a low-density crystal phase with a connected framework structure. We show that whereas amorphous ZrW_2O_8 has a structure that can be reconciled with a displacive-like phase transition from the crystal structure [1], [2], the structure of amorphous ZIF is more akin to a continuous random network that would only come from ZIF-4 via a reconstructive phase transition [3], [4]. As well as describing the phase transitions and structures of these two materials, we will discuss the implications of this work on PIA and TIA in general.

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Diffraction and nanoscale molecular electronic

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The Organic semiconductors are key components of photovoltaic cells, light-emitting diodes, and organic thin-film transistors. In these systems, knowledge of the molecular organization in the bulk, in the film, and in the interface region is crucial for any technological development. X-Ray Diffraction techniques have provided a host of information that guided the development of these devices [1].

Often it is impossible to grow crystalline samples of size and quality suitable for complete structural analysis. Less conventional structural powder diffraction methods, from which one can also retrieve otherwise inaccessible structural information, can come to the rescue. Grazing Incidence X-ray Diffraction (GIXD) gives information at nano-scale on the structure of films during the first stages of formation, as well as on their evolution during growth. X-Ray Reflectivity (XRR) measurements contribute to describe growth mechanisms (layer by layer or 3D) and monitor surface morphology.

Perylenes di-imide (PDI), and its derivatives, are considered most promising candidates for high performances organic electronics [2]. In order to establish the relationship between a PDI derivative film structure and its device performance, an assessment of the molecular arrangement was carried out by combining powder and thin film diffraction techniques. Moreover XRR performed *in situ* and in real time, during the high vacuum deposition, allowed us to identify the

structural and orientational transitions, which determine the charge mobility of the device. The role of temperature and the deposition flux on the growth mechanism were elucidated.

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Debye-Waller factor and thermal expansion in gold nanoparticles

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High q-space x-ray diffraction measurements are used to determine the Debye-Waller factor and the thermal expansion coefficient of Gold Nanoparticles of 2, 4 and 9 nm sizes. Bulk Gold was also measured for comparison purposes. Given the broad peaks present in nanoparticles, the solution to extract more information from the diffraction experiment lies in using the high q region of the diffraction pattern. In this work we measured the diffraction patterns up to 20 \AA^{-1} at 50, 150, 200, 250 and 300 K for each nanoparticle size. The diffraction patterns were then fit using the 15 K data as a 'model', so that only the Debye-Waller factor, the thermal expansion coefficient and a scale factor were optimized in a fitting code developed by the authors. The results show that the thermal expansion coefficient and the Debye-Waller factor depend on the nanoparticle size. The smaller the nanoparticle the smaller are both, the Debye-Waller factor and the thermal expansion coefficient. This surprising result could be explained by the strong surface effects present in the nanoparticles.

Keywords: gold nanoparticles, thermal expansion, Debye-Waller factor

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Debye function analysis on disordered metal-organic compounds: the pathfinder $[\text{Ru}(\text{CO})_4]_n$

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Several metal-organic compounds (such as, for instance, polymeric $[\text{Ru}(\text{CO})_4]_n$ [1]) show a peculiar form of anisotropic paracrystalline disorder where all Bragg peaks are dramatically broadened, except those along some axis – in this case the $h00$, $0k0$ and $00l$ peaks – which instead are sharp, as shown in figure. This kind of disorder is of high interest currently as it often occurs in Metal-Organic Framework materials (MOFs), a recent member of the smart materials family, and it relates to the actual display of the properties that make them attractive [2].