Rietveld refinement of single-crystal and/or powder Bragg diffraction intensities is a powerful method of elucidating the magnetic structure of magnetic materials; however there are inherent limitations in that Bragg intensities are sensitive only to the angle between the scattering vector and the spin orientations, rather than to the absolute orientations themselves. It is a direct consequence that a number of important problems in magnetic structure refinement (e.g. spin orientations in antiferromagnetic MnO) have remained unsolved. This talk will explore the possibility that local structure information contained in neutron total scattering data can help where average structure studies begin to fail - the idea being that local deviations from average structure allow some additional sensitivity via the magnetic diffuse scattering. The process of modelling this "local" information using atomistic reverse Monte Carlo methods will be discussed, with particular reference to its implementation in the program RMCProfile.

Keywords: reverse Monte Carlo, magnetic structures, diffuse scattering

## MS.61.5

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### An ion sputtering epitaxial FePt ultra-thin film studied by magnetic circular dichorism

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The best material for the future high density hard disk is the FePt alloy in a L10 ordered structure due to its high magnetocrystalline anisotropy constant and perpendicular magnetic anisotropy (PMA) property. Low energy ion assisted sputtering deposition of Fe/Pt multilayer was grown eptiaxially on the MgO(001) substrate. After annealing at 973 K, the order parameter reached above 0.95, the L10 ordered FePt film with growing along (001) orientation epitaxially was obtained. The out-of-plane MCD signals increases with increasing annealing temperatures. The out-of-plane orbital-to-spin ratio is found to be proportional to the order parameter. The strong interfacial hybridization between Fe and Pt layers produces enhanced perpendicular orbital moment in the L10 structure with strong PMA effect.

Keywords: magnetic film, magnetic behavior, ordering

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### Keeping a promise of the XFEL: Crystallography without crystals

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A primary scientific justification for construction of X-ray free electron lasers (XFEL's) has been the determination of the structure of non-crystallized macromolecules, such as proteins, from a set of diffraction patterns (DPs) obtained from randomly oriented single molecules exposed to ultra-short X-ray pulses [1]. It has been suggested that techniques akin to the method of "common-lines", developed for 3D electron microscopy, may be used to determine the relative orientations of the diffraction patterns. After orientation, the data from the DPs may be averaged to boost signal, and the electron density and hence molecular structure recovered by iterative phasing algorithms. We have recently demonstrated [2] that such methods can be used to recover the molecular structure in the absence of noise (i.e., at infinite signal.) However, the method breaks down for scattered photon intensities of less than about 10 per diffraction-pattern pixel. This is a far cry from the signal of ~ $4x10^{-2}$ photons per pixel expected from a typical 500 kDa protein. We describe progress in developing two algorithms for recovering protein structure from such extraordinarily weak signals: one based on the method of generative topographic mapping (GTM) [3, 4]; and one on the exploitation of the symmetry of the random orientations of the copies of the molecule.

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Keywords: XFEL, orientation and averaging, real space direct method

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### Hybrid thresholding-projection algorithms for the crystallographic phase problem

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With the ideal algorithm, success in phase retrieval would depend solely on the prior knowledge of the object to be reconstructed and the quality of the data collected. For ab-initio phasing, which does not rely on prior information other than the fact that an object is made of a finite number of atoms, or it has a finite extent, two forms of algorithms have been developed in parallel. By doubling the Bragg sampling, increasingly sophisticated iterative projection algorithms [1] have demonstrated practical solutions to giga-element nonlinear phase retrieval problems, escaping local minima and producing images at resolutions beyond the capabilities of lens-based optical methods without the need for atomic resolution data. These methods have enabled the birth of diffraction microscopy, a.k.a. lensless imaging, a technique whereby the image of an object is obtained by computational phase retrieval of a diffraction pattern instead of using a lens to transform the pattern into an image The adaptation of these algorithms to crystallography have lagged -so far- due to sub-Nyquist sampling imposed by the crystal periodicity. Contrary to conventional wisdom, these algorithms can be adapted to allow for accurate and robust reconstruction from a number of measurements dictated by the signal's structure rather than its (finite) extent.

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