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A ray tracing method for predicting contrast in neutral atom beam imaging

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ABSTRACT

A ray tracing method for predicting contrast in atom beam imaging is presented. Bespoke computational tools have been developed to simulate the classical trajectories of atoms through the key elements of an atom beam microscope, as described using a triangulated surface mesh, using a combination of MATLAB and C code. These tools enable simulated images to be constructed that are directly analogous to the experimental images formed in a real microscope. It is then possible to understand which mechanisms contribute to contrast in images, with only a small number of base assumptions about the physics of the instrument. In particular, a key benefit of ray tracing is that multiple scattering effects can be included, which cannot be incorporated easily in analytic integral models. The approach has been applied to model the sample environment of the Cambridge scanning helium microscope (SHeM), a recently developed neutral atom pinhole microscope. We describe two applications; (i) understanding contrast and shadowing in images; and (ii) investigation of changes in image formation with pinhole-to-sample working distance. More generally the method has a broad range of potential applications with similar instruments, including understanding imaging from different sample topographies, refinement of a particular microscope geometry to enhance specific forms of contrast, and relating scattered intensity distributions to experimental measurements.

1. Introduction

Neutral atom beam microscopy is an emerging technique that uses a focused or collimated beam of neutral atoms, principally helium, as a microprobe. The atom beam is typically fixed and the sample position is rastered. Atoms scattered in a particular direction are counted and used to build up a 2D micrograph, in a process similar to the operation of many other scanning microscopes. The method has considerable promise for non-destructive, exclusively surface sensitive, imaging of delicate samples within both the physical and biological sciences and for the formation of images with novel forms of contrast (Barr et al., 2016, 2014; Fahy et al., 2015; Koch et al., 2008). In helium images acquired to date, contrast appears to arise predominantly from variations in diffuse scattering due to the local surface structure ('topographic' contrast (Barr et al., 2016)) and is analogous to the established technique of secondary electron emission in SEM. However, at present there is no consistent method for predicting or understanding that contrast. With emerging evidence for chemical contrast (Barr et al., 2016) and the potential for diffractive and interference contrast, it becomes important to understand which features in images can be explained purely by diffuse scattering through sample topography.

Presented here is the development of a computational framework to construct topographic contrast in a scanning helium microscope (SHeM) from a 3D model of the sample and signal collection environment. Ray tracing is used as the basis of our approach, treating helium atoms as classical rays that travel in straight lines. Compared to alternative techniques, such as wave propagation simulations, ray tracing is computationally inexpensive while still being able to capture phenomena such as multiple scattering. Multiple scattering is particularly important in neutral atom microscopy since helium atoms, unlike electrons or photons, are not absorbed or collected within the sample region. Beam atoms may therefore scatter multiple times from the sample and its surroundings, while still continuing to be detected. These multiple scattering processes can cause unexpected features in images, such as diffuse illumination (Witham and Sanchez, 2014); and could not be properly modelled using integral models (Hedgeland et al., 2005). Any integral model would have to be reformulated for each new geometry and would become computationally more expensive as the number of included scattering events increases, hence we consider them impractical for our needs. Ray tracing also allows the use of arbitrary sample geometries, thus it would be possible to use quantitative surface profileometry to generate the sample surface for simulation in future work. Quantum interactions with the sample are neglected, since it is known that the scattering of helium from all but the cleanest surfaces is largely diffuse (Engel, 1978; Poelsema et al., 1982).

The simulation framework was developed in house allowing

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complete control of the scattering process, including defining the incoming helium beam profile, the sample geometry and the detection conditions. The source code is made available by the authors Lambrick (2018). Diffuse scattering was modelled using a specified angular distribution centered on the surface normal (typically a cosine distribution), enabling topographic contrast to be generated from an arbitary sample profile. In principle, angular scattering distributions from the sample can be varied with spatial position, therefore enabling investigation into chemical effects. Rays scattered into a particular collection aperture were counted, enabling images to be constructed in exactly the same way as in the physical instrument. In addition the approach can be used to investigate instrumental factors such as the transmission of atoms through a particular detection geometry, and the consequence in images of the effusive beam components that have been seen in previous work (Fahy et al., 2015). The framework is currently optimised for the Cambridge SHeM, and can easily be adapted for similar atomic beam instruments.

The remaining paper is organised as follows. Section 2 discusses the Cambridge SHeM, ray tracing methods, and how these are related to the current work. Section 3 details the implementation of the simulation. Section 4 presents an illustrative comparison between experimental and simulated images, and explores the utility of the simulation for characterising collection aperture transmission probabilities in the SHeM. Finally, Section 5 gives a summary and outlook.

2. Background

2.1. Main SHeM components

Scanning helium microscopy uses a collimated thermal energy helium beam as a probe that is rastered over the surface of a sample, to create a spatially resolved image. Fig. 1 shows the main elements of a typical SHeM instrument; a more detailed description can be found in Barr et al. (2014). The helium beam is first produced by supersonic expansion of high pressure helium gas into a vacuum (Scoles, 1988). The centreline of the expansion is passed through a skimmer, then a pinhole collimates the beam to form the microprobe. Beam-widths of ~1 μm (Eder et al., 2012) have already been demonstrated by using Fresnel zone-plates and there is a roadmap to achieve a usable resolution of ~50 nm in the next generation of SHeM. Similarly, a resolution of 350 nm has been reported by using using very small working distances, 10–30 μm (Witham and Sanchez, 2012, 2011). Atoms within the microprobe are scattered by the sample, depending on the local beam-surface interaction. Images are then constructed by rastering the sample in the beam, while detecting the helium intensity passing through a detection aperture in a particular direction, using a custom high sensitivity helium detector (Alderwick et al., 2008). The 'brightness' of each pixel is proportional to the number of helium atoms detected while the sample is in a particular position.

For contrast prediction, the exact details of the source and detector need not be considered. The lower section of Fig. 1 shows an enlarged view of the sample region, containing the most important elements for the present simulation framework. These include the 90° total scattering geometry and 45° angle of incidence, the exact positioning of the pinhole and detector apertures, and the extent of the solid geometry surrounding the measurement area. Usually, the beam is incident on the sample at the point of co-incidence between the incoming beam and the outgoing detector cone.

2.2. Diffuse atom surface scattering

Unlike in charged matter microscopy, where there is significant penetration into the surface, thermal energy helium atoms scatter as a result of the repulsion between the valence electrons in the scattering atom and the valence electrons in the surface (Farias and Rieder, 1998). There is no penetration into the bulk, hence it is only necessary to define how atoms in the simulation respond to scattering from the topmost electronic surface of the sample. For scattered helium atoms the outgoing direction could be specular (Politano et al., 2011), a diffraction pattern (Traeger, 2006), involve rainbow effects (Miret-Artés and Pollak, 2012), or diffuse scattering (Poelsema et al., 1982).

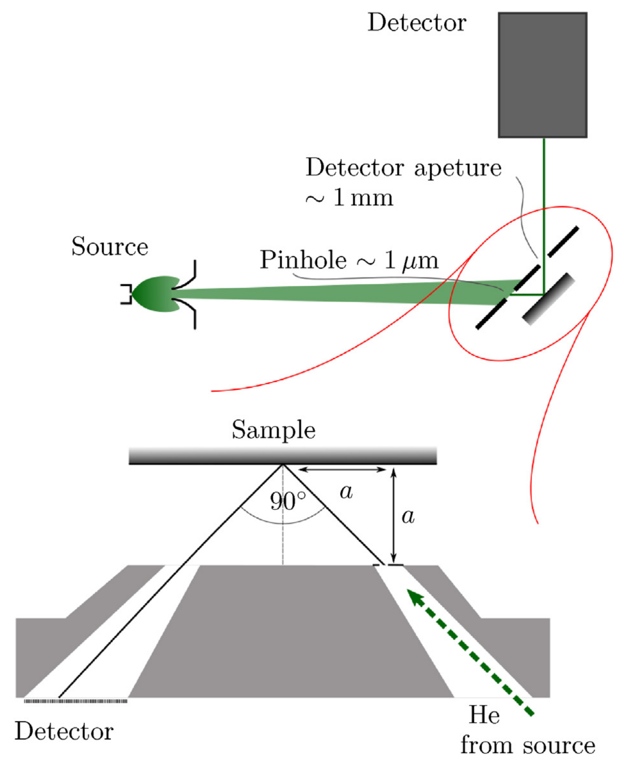

Fig. 1. Simplified schematic of a scanning helium microscope (SHeM), showing the principle of operation. The helium beam is formed in a supersonic expansion, then collimated by a skimmer and pinhole. Atoms scatter off the sample and those that enter the detector are counted. The image is formed by rastering the sample position. The close up shows the key parts of the instrument that are relevant to the current simulation framework, including the sample position and the mounting plate for both the pinhole and detector apertures. In the current Cambridge SHeM configuration $a \approx 2.1$ mm.

Any randomness of the surface on a length scale between the wavelength of the atoms and the beam width (which spans 4 orders of magnitude) will have an effect on the observed scattering distribution, which is then averaged over the area of the beam. For scattering from such 'rough' surfaces, the averaged scattered direction is expected to be independent of incident direction, and to correspond to a normally centred cosine distribution (Greenwood, 2002). Since we are focussing on the generalised 'topographic contrast' associated with most 'real' surfaces imaged using SHeM, the framework presented here uses that normally centred cosine distribution. The intensity scattered into an infinitesimal solid angle, dΩ, in a particular direction defined by the polar angle to the surface normal, θ, and the azimuthal angle, φ, is given by

$$I(\theta,\varphi)\,\mathrm{d}\theta\,\mathrm{d}\varphi = \frac{\cos\theta\,\mathrm{d}\Omega}{\int_{2\pi}\cos\theta\,\mathrm{d}\Omega}, \tag{1}$$

where the integral normalises the distribution over the outgoing half-space. Given that $\mathrm{d}\Omega = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi$, we can substitute and integrate to obtain the azimuthally independent result

$$I(\theta) = \frac{1}{\pi}\sin\theta\,\cos\theta. \tag{2}$$

Note that the cosine scattering distribution is independent of incident direction. Fig. 2 shows the cosine distribution of scattered atoms, and indicates the selection of some of those atoms by a detector cone to