Optimal Sampling and Reconstruction Strategies for Scanning Microscopes

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Abstract

Images from scanning transmission electron microscopes are now used routinely to quantify the morphology, structure, composition, chemistry, bonding, and optical/electronic properties of nanostructures, interfaces and defects in many materials systems. However, quantitative and reproducible observations for many materials of current technological importance are limited by electron beam damage destroying the sample before the highest resolution information is obtained. The aim for broadening STEM applications to a wider range of samples and processes is therefore now to focus on more efficient use of the dose that is supplied to the sample. In practice, this is achieved by minimizing the experimental dose, dose rate and dose overlap for any image, resulting in a new approach for dose fractionation and optimizing the data content per unit dose – reducing the number of pixels being sampled, and using inpainting /machine learning methods to reconstruct the images. Here, the basic approach to integrating of sub-sampling/inpainting/compressive sensing and machine learning into conventional STEM imaging/spectroscopic hardware (and all other scanning systems) will be described and the potential for future developments will be discussed.

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1. Introduction

The advent of aberration corrected STEM [1,2] has led to an unprecedented increase in the achievable spatial resolution from all forms of imaging and spectroscopy (Z-contrast, Annular Bright Field, EELS, EDS etc.), but this has also been accompanied by a simultaneous increase in the operational probe current under typical imaging conditions. While the increased current is advantageous for observations of atomic scale dopants in some samples, typical electron doses are now several orders of magnitude higher than many materials can withstand [3]. Dose considerations have now become the most critical experimental parameters when imaging beam sensitive materials, which usually leads to a practical reduction in the electron dose and dose rate being implemented at the cost of decreased signal-to-noise ratios and a poorer spatial resolution than the microscope is capable of delivering at the higher dose/rate levels. In this paper, we examine the main issues associated with minimizing beam dose in the STEM (and as the methodology is essentially the same in all scanned methods, this applies to any other scanned imaging system) and propose the use of a sub-sampling and inpainting methodology (generally falling within the mathematical field of compressive sensing) as a method to overcome the effects of the beam, leading to an improvement in the resolution and reproducibility of high resolution analyses [4-8].

2. Practical Scanning Systems

In a standard STEM, the way the scan system usually works is that it moves the beam from left to right across a single row with a dwell time (typically ~5μs) for each pixel in that row (Figure 1). At the end of the row, the beam flies back to the left-hand-side, moves down one pixel and then completes a row again (this is like the way a traditional typewriter used to work or an older cathode ray tube (CRT) television). After the flyback, the beam typically has a longer dwell time at the left-edge to allow for any hysteresis in the scan to damp out and the left-edge of the scan to be aligned at the same location for each row. The beam size is typically the same regardless of the magnification of the image, which can be as small as ~0.1nm for an aberration corrected (Cs-corrected) STEM [7,8]. In a low magnification image, the area of the scan is large and the pixel size is therefore much larger than the size of the beam. For example, if we continue our discussion for a Cs-corrected STEM, in a 1000 x 1000 pixel scan covering 1mm x 1mm of sample, the pixel size is 1μm, i.e. 1000 x the size of the beam. To achieve atomic resolution, the magnification of the microscope is increased to the point where the pixel size approaches the atomic separation, i.e. ~0.1-0.5nm. For many of the most impressive atomic resolution STEM images that have been obtained from beam stable samples, the magnification is turned up to a level where the pixel size is actually much smaller than the probe size, leading to an oversampling of the image.

When an SEM/STEM is running at low-magnification, beam damage is typically not an issue that any experimentalist has to face, as the distance between the beam locations is very large, and the likelihood that the scan hits exactly the same location in successive sweeps is very small – damage still occurs, but it is below the scale of the intended image resolution. It is only when the beam and pixel size starts to overlap that the damage becomes serious, and this is of course the condition that the microscope aims to achieve for the highest spatial resolution (Figure 1). If we think about the problem from the perspective of overlapping beam positions and their effect on the measurable damage, then it is clear that if we can increase the spacing of the beam positions at high magnification then we will be able to avoid/reduce the beam damage problem that plagues high resolution SEM/STEM (Figure 1). Of course, the issue with this "sparse sampling" approach is that we would then need a means to "reconstruct the full image" from this sub-sampled acquisition. As the quality of the image then would obviously depend on how much sampling was included, the best or optimal sampling would be the one where the physics of the beam damage process was minimized and the ability to reconstruct the image was maximized.

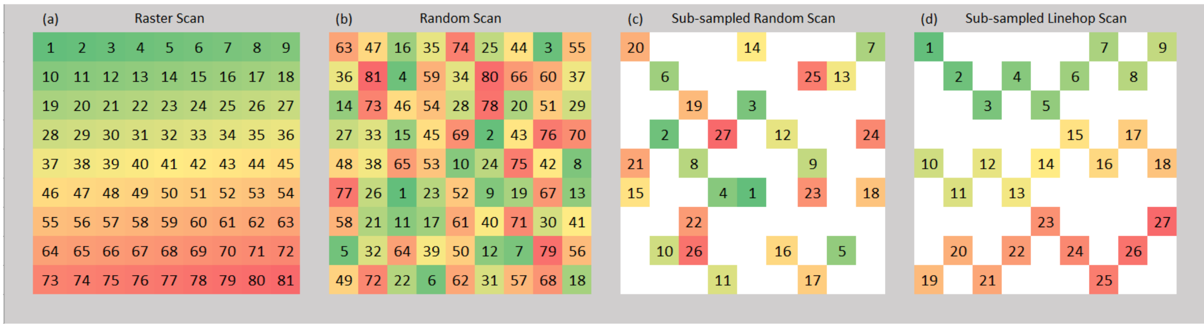

Figure 1: Examples of various scanning patterns in a 9x9 grid. Number and colour indicate scanning order. (a) Raster scanning is the traditional method of scanning in STEM. (b) Space filling random scanning has been shown to reduce beam damage in beam sensitive samples [8]. (c, d) Two scanning patterns possible using probe sub-sampling; sub-sampled random scanning and sub-sampled linehop scanning at 33.3% sampling ratio.

3. Sub-sampling and Image Reconstruction

As we can see from Figure 1, it is possible to obtain a scanned image by using both a set of “random” beam positions, and a “random walk” or “line-hop” scan. Practically, the line-hop approach is easier to implement on electron microscopes as it avoids much of the hysteresis issue present in conventional scanning systems, permitting the system to run at the fastest possible speed [5]. Implementation of the line-hop on any electron microscope can be achieved by plugging into the external scan port on the microscope and implementing a signal generator to create the scans and record the images [5]. In view of its simplicity to implement, in the remainder of this paper we will discuss the implementation and application of this line-hop method (please note that it is possible to design a hardware solution to reduce hysteresis and permit true random scanning, but such a solution is not retrofittable to existing systems).

The key challenge for all sub-sampling methods is to reconstruct the sub-sampled image. Compressive sensing and/or Inpainting is a method of efficient signal acquisition and reconstruction via the solving of a set of undetermined linear equations [9]. Like traditional image compression techniques, it relies upon the fact that given an appropriate coordinate system (or ‘Dictionary’), complex high dimensional signals such as an image can be expressed within a margin of error by a (potentially) much smaller set of parameters, describing a linear combination of signal patterns with their respective scalar coefficients. The goal for any image reconstruction is to form a complete signal (with the smallest error) from as few measurements as possible. As an example of this process, consider the case of a simple 1-dimensional (1-D) signal, such as a wave shown in Figure 2. Here, a series of dictionary elements (in this case Fourier components) can be used to re-construct a true signal (Figure 2b). But now what happens if we do not measure the complete signal? Figures 2 c-f show the effect of sub-sampling the true signal. For relatively high levels of sub-sampling (missing only a minimal amount of information), it is clear that we can fit the dictionary elements to the observation, effectively “inpainting” the missing level of sampling in our experiment. As we reduce the level of sampling, the ability to “fit” to the data with a minimal error is reduced, until when we get to only 2.5% of the data, the error is unacceptably large. However, given that the damage induced in the sample is a function of the speed of the scan, and the overlap of the beam positions, reducing the overall number of beam positions in the image can have a tremendous effect on the overall sample stability during the experiment. It is also important to note that there are many possible algorithms for the reconstruction of these sub-sampled images, and more are being developed daily. All of the existing algorithms use the same construct to inpaint the image and so once the hardware solution is in place, the methodology can improve with every algorithm upgrade.

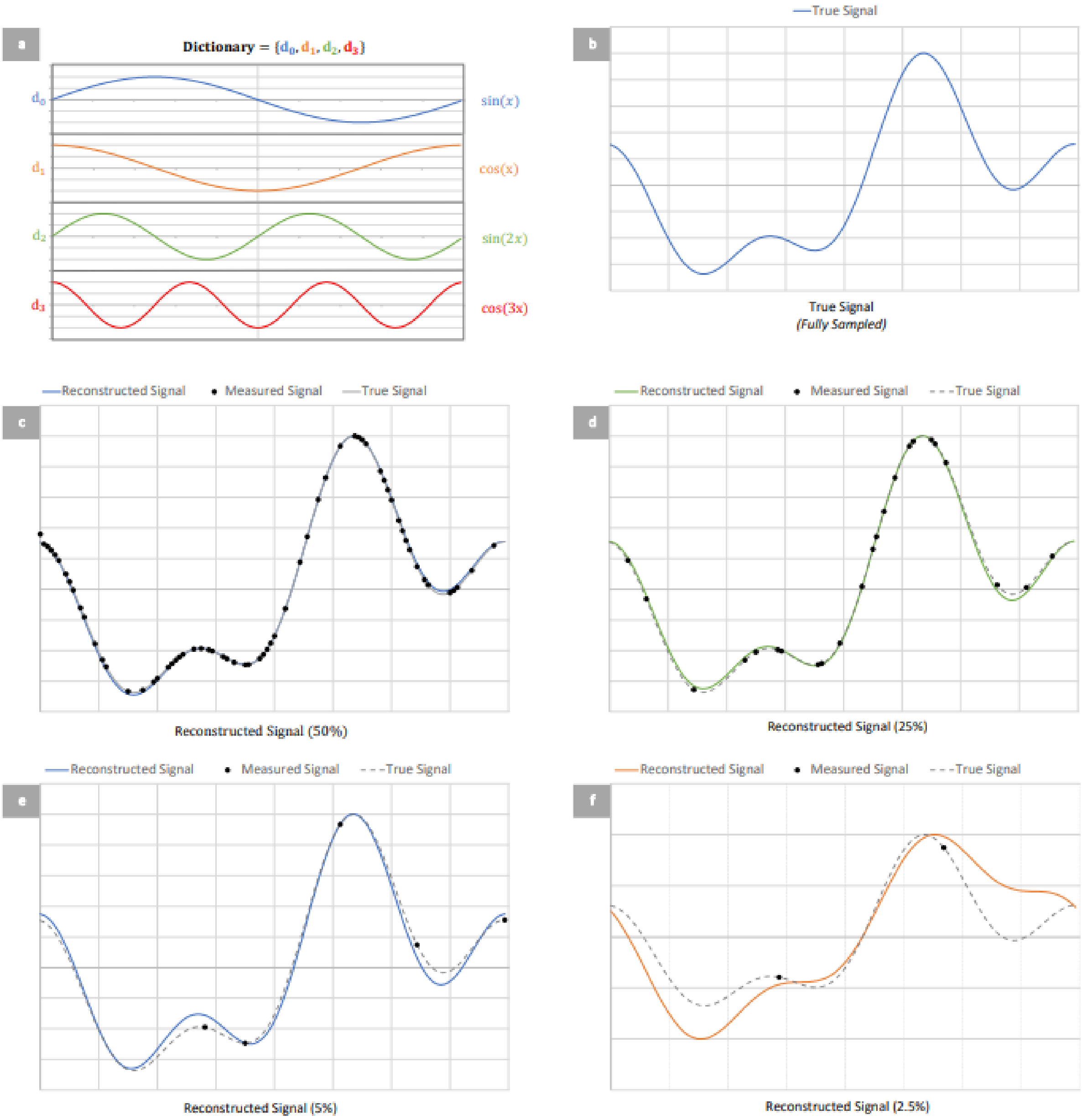

Figure 2: (a) A series of dictionary elements (Fourier components in this case) can be combined with defined scalar weightings to reproduce the true 1-D signal (b). By reducing the number of points in the true signal (c-f) we can increase the speed and decrease the dose in the sampling of our experiment, but still generate a good fit to the data. At some point (f) the level of sub-sampling leads to an unacceptable error in the reconstruction. This level of sub-sampling is material and instrument resolution dependent [8].

3. Example Reconstructions

There is not enough space in this brief publication to go through the details of the reconstruction algorithm that we will use. Here we will simply state that we are using the Beta Process Factor Analysis (BPFA) approach to inpaint sub-sampled images [8,10,11] and show a few examples of the use of these methods. In the use of the BPFA methodology there are a number of tunable parameters that are used to increase the efficiency of the algorithms to reconstruct the images. Again, in this publication, we cannot go through all the details of the processes involved, but will simply show the results and refer the reader to other publications that discuss the methodology involved [4-8]. The first example, we show is the reconstruction of the famous “Barbara” image. Figure 3 shows the original image sub-sampled to 25% and reconstructed using BPFA. The two example reconstructions highlight the “tuning” of the reconstruction parameters that can be achieved and the quality of the retrieved image.

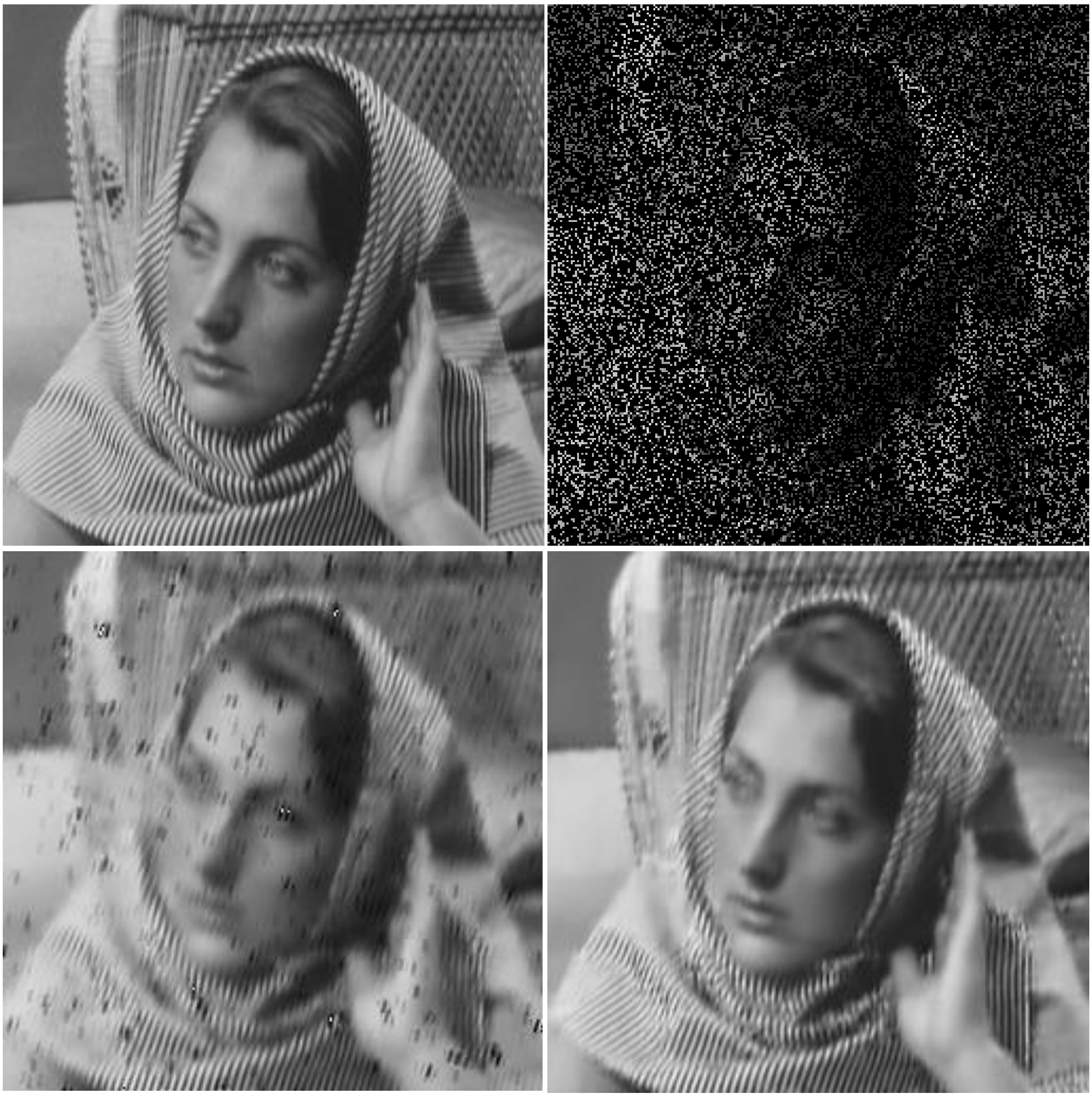

Figure 3: (a) Public domain test image, 'Barbara'. **(b)** 25% randomly subsampled image of 'Barbara'. **(c)** Reconstruction of **(b)** with deliberately poor reconstruction parameters and **(d)** Reconstruction of **(b)** with optimised reconstruction parameters.

The example shown in Figure 3, involves an image that has been acquired fully sampled and then sub-sampled for demonstration purposes. The final example we will show is of an image reconstructed from an experiment where the image was acquired as a sub-sampled image and then reconstructed. Figure 4 shows a traditionally acquired atomic resolution Z-contrast STEM image of Ceria, a 6.25% sub-sampled line-hop image of the same sample in the same position (beam damage is not an issue at these doses for this sample), and the reconstruction performed on the aforementioned sub-sampled image. To determine the accuracy of the reconstruction figure 4c is compared to figure 4a by two metrics; peak signal-to-noise ratio (PSNR) and cross correlation. Figure 4c has a PSNR of 20.6752 dB and a maximum cross correlation of 0.75037 when compared to figure 4a, both of which fall within acceptable limits for interpreting the image directly. This approach increases the speed of the acquisition by 16x while reducing the overall dose by the same amount, and yet the quality of the image is essentially the same.

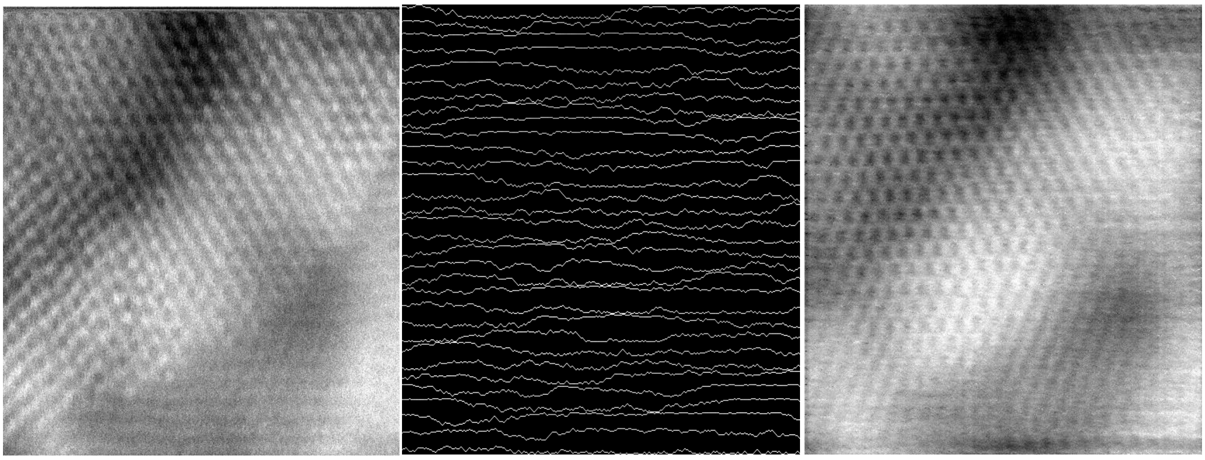

Figure 4: (a) 512 x 512 fully sampled atomic resolution Z-contrast image of Ceria. (b) 6.25% sub-sampled line-hop image acquired with the same beam conditions at the same location and (c) reconstruction of the 6.25% sub-sampled image using BPFA.

4. Conclusions

The results discussed in this paper demonstrate that it is possible to determine an optimal approach to forming the most efficient image in any scanned imaging system. By moving beyond hardware only defined solutions for imaging beam sensitive samples and employing compressive sensing/inpainting/machine learning methods to reconstruct images that are sub-sampled, we can increase the spatial and temporal resolution of images. This approach opens up a wide range of materials and dynamic processes that can now be studied by electron microscopy and other methods. As the analysis so far has only focused on employing these AI methods to the analysis of single images with BPFA, there is potential to extend the resolution limits for imaging even further in the future as more images of different samples are included in a training data set and using learning algorithms to improve reconstruction quality. In addition to increasing the efficiency of the algorithms for the analysis of particular image/scattering processes in electron microscopy, we can develop an overall workflow that will improve imaging capabilities across multiple techniques (this workflow and the application software is currently being developed by Nuxutra). Figure 5 shows how the incorporation of different imaging methods into the workflow can bring multi-scale, hyperspectral measurements into the training datasets and these complete analyses can then be used to improve the resolution of wide-ranging expensive, difficult to use and over-subscribed scientific instrumentation that is the bedrock of the development of new advanced materials.

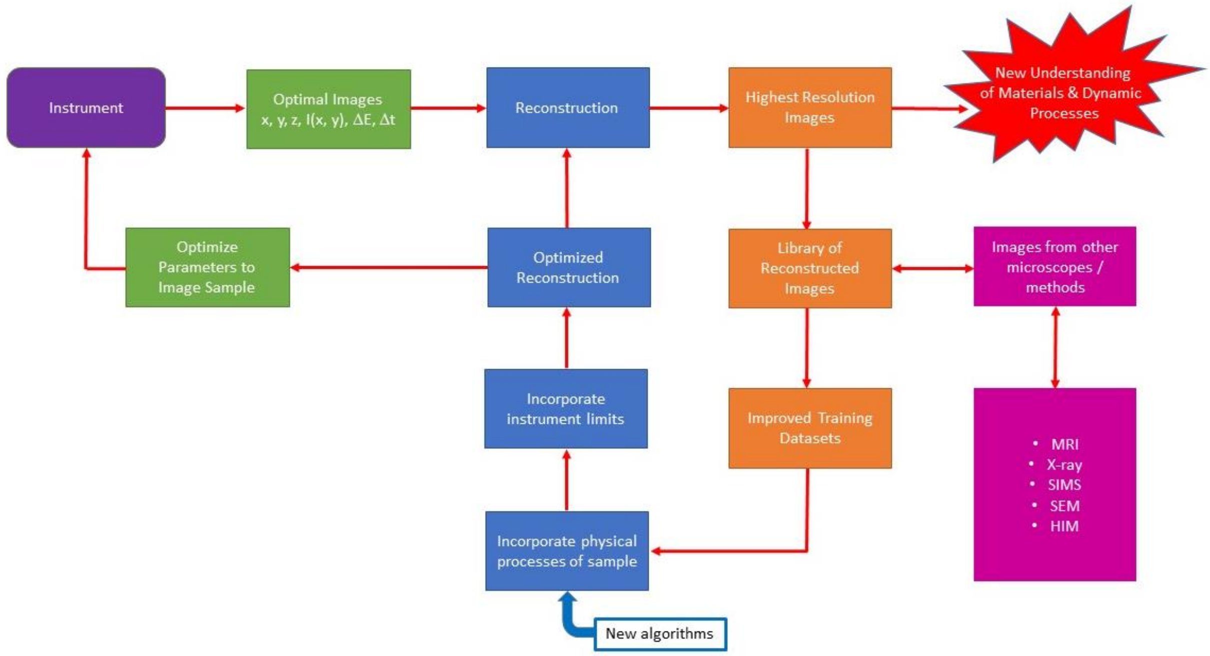

Figure 5: The physics of beam interactions can be incorporated into sampling strategies for many experimental methods, optimizing the use of each method individually and enhancing the scientific information obtained from the methods used together to solve materials challenges.

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