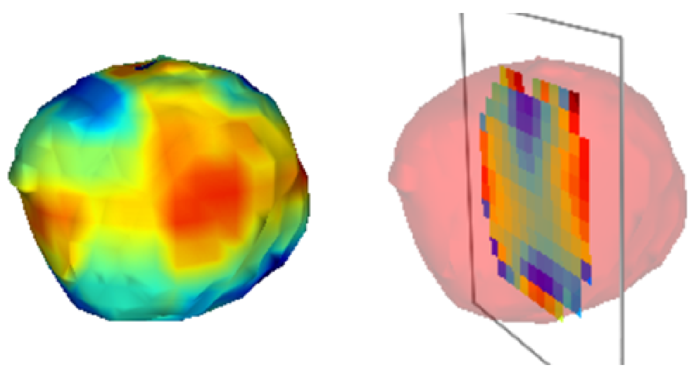
Making the Most of Rock and Roll

An iterative algorithm that can account for uncontrolled motion of nanoparticles enables imaging of this tiny system via Bragg coherent diffraction.

By Marric Stephens

Determining strain in nanoparticles is tricky at the best of times. It's even harder when the particles won't stay still. This issue is particularly acute for Bragg coherent diffraction imaging (BCDI) of nanoparticles, where smaller particles are more likely to pitch and roll unpredictably because of radiation pressure. Now, Alexander Björling of Lund University, Sweden, and colleagues turn this uncontrollable motion to their advantage with an algorithm that can piece together the strain field for particles that rotate around unknown axes [1]. The method could make BCDI applicable to smaller nanoparticles than ever before.

In conventional BCDI, a coherent x-ray beam illuminates a nanoparticle from multiple angles sequentially. The diffraction pattern acquired at each angular position constitutes a slice through the sample's Fourier representation. By combining and inverting these slices, researchers can gain a 3D picture of the strain-induced distortions and defects in the particle's crystal lattice. For smaller particles, only very intense x-ray beams can produce the necessary diffraction patterns, but such beams jostle the particle even more severely.



Credit: A. Björling *et al.* [1]

In the new approach, instead of turning the sample manually through controlled angular steps, they exploit the uncontrolled rotation induced by the beam. Using an iterative likelihood-maximization algorithm, the researchers derive a "best-guess model" of the particle's diffraction volume based on slices captured at unknown orientations. The only prior information required is the rough size of the particle, which is easy to estimate.

Björling says that one of the most interesting potential uses of this technique would be studying catalytic nanoparticles, which can be more effective catalyzers when strained. But until now, the 10-nm particles typically used as industrial catalysts have been too small to characterize using BCDI.

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REFERENCES

1. A. Björling *et al.*, "Three-dimensional coherent Bragg imaging of rotating nanoparticles," **Phys. Rev. Lett. 125, 246101 (2020).**