Scaled-up Diffraction of Crystals and Helixes

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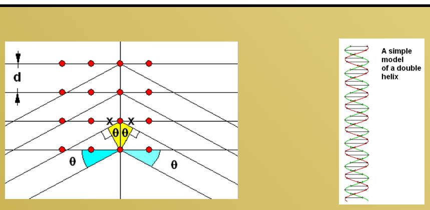
BACKGROUND

Diffraction experiments using X-rays on crystals showed one of the first convincing pieces of evidence that matter is composed of atoms. They also showed that, in crystals, atoms are ordered in repeating arrangements that produce diffraction peaks at certain angles of orientation. Bragg diffraction experiments with X-rays are performed routinely by students in the laboratory to observe these effects. Scaled-up versions of the experiment, using microwaves or visible light instead of x-rays, are also useful in gaining insight in the experiment and learning the laws of diffraction.

We find that adding a simulation to the experimental data adds a more complete understanding of the diffraction phenomenon and makes the experiment richer in physics. In what follows we describe an experiment with microwaves where the crystal is a macroscopic lattice of steel spheres and an experiment with visible light diffracted off a thin wire given the shape of a helix.

PURPOSE AND HYPOTHESIS

Diffraction patterns were simulated and obtained for scaled-up crystals and helixes. Microwaves and visible light were used instead of x-rays. Surface and finite size effects are noticeable in the data and provide additional insight in the diffraction observations.



Geometry of the Bragg diffraction experiment and the double helix.

Experimental results and simulations

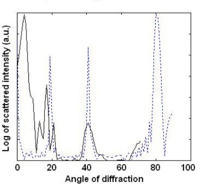
The diffraction peaks expected from an infinite crystal are the ones that satisfy Bragg's law:

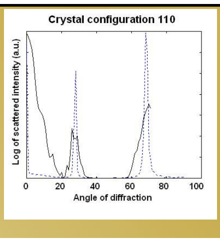
$$2d\sin\theta = n\lambda$$

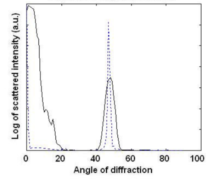
Where λ is the wavelength of the scattered radiation and n is an integer.

But in the actual data obtained with a finite crystal in the laboratory, the peaks are broad and have additional structure in places that do not satisfy the Bragg condition. This is shown in the figures below as the black solid lines. To understand this observation we ran simulations of the scattering process.

First we simulated the case of a very large crystal (large in the sense of many atoms) and scaled to have short wavelengths. This first simulation, using 32,768 atoms and a wavelength of 420 microns reproduced the expected peaks with much less structure. This is shown in the figure as the dashed blue lines. The figures show three configurations 100, 110 and 210 corresponding to orientations of the crystal at 0°, 45° and 27°.



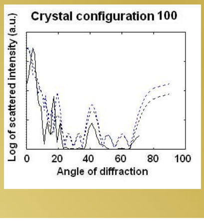


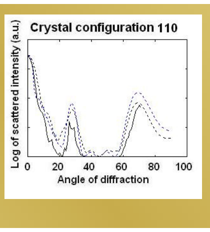


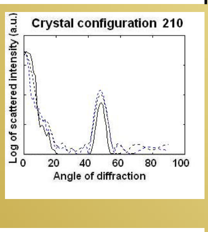
Observing the discrepancy between simulation and actual data, the natural question to ask is whether the additional structure observed in the experiment is due to the finite size of the crystal (only 64 scattering "atoms") or the fact that the wavelength and size of the crystal are macroscopic as compared with the size of the experimental apparatus.

Finite size effects and comparison with simulation

To gain insight in what is causing the discrepancy, we simulate the experiment with the correct number of "atoms" (only 4x4x4=64) and the correct wavelength, which is 2.6cm. In this more realistic simulation the experiments approximate the theory much better as observed in the following figures. The theory is shown as the dotted black line and the actual data as a solid black line.







We also ran a simulation where the size of the crystal is scaled down to microscopic dimensions as well as the wavelength of the radiation used. The results are shown as the blue dotted lines in the figures above. The approximation is still good in this case, so we can conclude that the main cause of the discrepancy between the perfect textbook example of Bragg diffraction and the scale up version doesn't come from the physical size of the crystal and wavelength, but rather to the finite number of scattering "atoms".

This should apply to X-ray diffraction of nanocrystals, where additional structure should be expected.

Work in progress

Diffraction of Helixes Using Visible Light

In a similar fashion, as in the Bragg diffraction experiments it is possible to scale up the diffraction off a helix. The famous X-ray diffraction picture of DNA taken by Rosalind Franklin helped elucidate the structure of the molecule and it showed a distinctive X pattern of interference fringes. The scaled-up version of the experiment that we use employs a He-Ne laser as the source and a thin wire as the helix. Initially only a single helix is employed. Below are our preliminary results:

Compare this diffraction pattern with the one of DNA taken in 1952 and published in Nature by Franklin and Gosling, sometimes called "Photo 51"

References

1) Microwave Bragg Diffraction Apparatus, Harry F. Meiners, Welch Scientific Company, Cat. 2641
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3) The optical activity of Oriented Copper Helices. I. Experimental. Ignacio Tinoco, Jr., and Mark P. Freeman, Vol 61, pages 1196-1200