

Solving the phase problem in x-ray diffraction

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(PhysOrg.com) -- Nearly 100 years ago, in 1912, a paper by Max von Laue made it possible to use x-rays to study the structure of different crystalline substances. He won a Nobel Prize in 1914 for his work, but, even so, the method was limited. Without being able to measure the phases of the diffracted beams, it is only possible to use Laue's method to get a partial description of material structures.

"While Laue's work was very important, it doesn't provide the complete picture," Emil Wolf tells *PhysOrg.com*. "Even though we have an idea of how DNA and other substances are structured, thanks in part to this process, it is really an approximation. There is actually data missing to give us a complete picture of many of the structures we are familiar with."

Wolf is a researcher at the University of Rochester in Rochester, New York. He shows that by reformulating the problem of phase measurement in diffracted x-ray beams, it might be possible to better study the structures of many materials, providing a more complete picture. "Instead of trying to measure beam phases - something that is practically impossible and meaningless," Wolf points out. "One should measure instead certain correlations collected with averages." His efforts are reported in *Physical Review Letters*: "Solution of the Phase Problem in the Theory of Structure Determination of Crystals from [X-Ray Diffraction](#) Experiments."

"Part of the problem is that many assumptions are made based on an

idealized version of a beam,” Wolf continues. “Unfortunately, the usual assumptions are unrealistic. Beams are not monochromatic; they are irregular. Instead of trying to make [impossible] measurements of erratic phase variations or estimating it with an idealized rendition, we propose using measurable [correlation](#) functions to obtain the missing data.”

Having the ability to more accurately probe the structures of many materials could be useful going forward from a fundamental standpoint as well as a practical standpoint. “Great recognition has been given for just approximations. Having more complete structures could be even more helpful. For medicine and chemistry, this would be helpful because in order to make improvements to drugs, you want to know how the atoms arranged. This could have great implications in physics, chemistry and medicine as well,” says Wolf.

The next step, Wolf says, is to prove his work experimentally. He has done a great deal of work to study the feasibility of testing out his equations and methods, and he feels that it is something doable. “There has been some interest from experimental groups and other researchers who want to try this out. There are some facilities that are equipped to try this out. It may take some time to work out how to do it, but it is only a matter of time.”

Wolf continues: “I’ve been examining some of the literature, and it appears that it is possible. What we’ve come up with measuring beam correlations offers a new principle for a more complete solution to a very basic problem. It may take some time before other scientists appreciate these results, but this issue is too important and this solution has too much potential to be set aside.”

More Information: Emil Wolf, “Solution of the Phase Problem in the Theory of Structure Determination of Crystals from X-Ray Diffraction

Experiments,” *Physical Review Letters* (2009). Available online:
<http://link.aps.org/doi/10.1103/PhysRevLett.103.075501>.

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