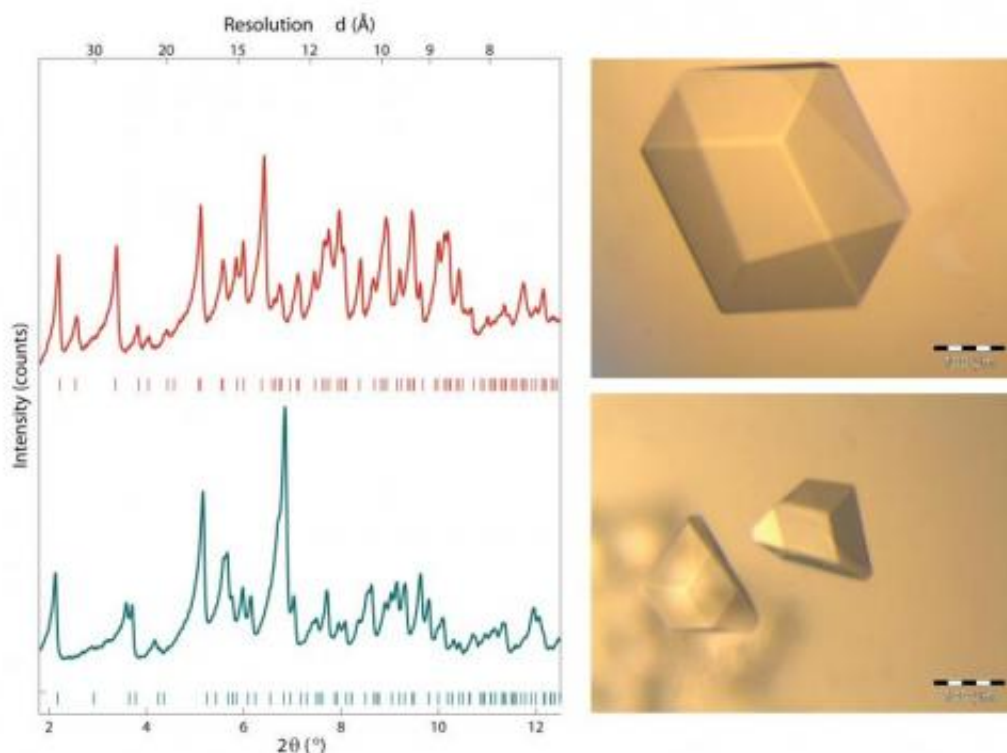


Chemist develops X-ray vision for quality assurance

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Two different crystal forms of the protein insulin. The illustration to the right shows two different crystal forms of insulin using single crystal diffraction, while the graphs to the left present two different insulin ‘fingerprints’ taken using powder diffraction. Credit: Technical University of Denmark

It is seldom sufficient to read the declaration of contents if you need to know precisely what substances a product contains. In fact, to do this

you need to be a highly skilled chemist or to have genuine X-ray vision so that you can look directly into the molecular structure of the various substances. Christian Grundahl Frankær, a Postdoc at DTU Chemical Engineering, is almost both, as he has developed a method that allows him to use X-rays to look deep into biological samples.

The 'Fingerprints' of a Substance

The technique is called 'powder diffraction' and involves subjecting a sample to an intense beam of X-rays. When the beam hits the sample, it disseminates in the same way as light does when reflected by a disco ball. This generates a pattern that reflects the structure of the material. Each individual substance has its own unique pattern—a kind of 'fingerprint'—which makes it readily identifiable when the results are run through a database.

Powder diffraction is currently used to identify simple substances such as sugar, salts and minerals, but the idea of using the same technique to characterize advanced biological molecules such as proteins is truly innovative. It is for this reason that the method has enormous potential in both food production and the pharmaceutical industry, where more and more attention is being devoted to [protein](#)-based medicines.

"I have tested different types of infant milk formula, protein powders and detergents. By taking a small sample of powder and bombarding it with X-rays, I can determine what substances the powder contains—and in what concentrations—within ten minutes. In addition, the analysis will typically reveal some information about how the product was made," relates Christian Grundahl Frankær. The method is therefore ideal for quality assurance of new products on the market.

Crystal Forms Determine Properties

Proteins are large molecules with complex 3D structures. The shape of a protein—or its crystal structure—can significantly alter its properties. A protein such as insulin may have many different crystal forms, and the form the substance appears in may affect its solubility or level of activity. This, in turn, may be of significance to how the protein will react when it enters the human body. For this reason, it makes a lot of sense to analyse the crystal forms of different proteins both during production and in the quality assurance of protein-based medicines, but this has simply not been practical nor financially viable until now. Christian Grundahl Frankær explains:

"We have now demonstrated that [powder diffraction](#) can actually be used on biological substances such as proteins. The results are not as detailed as in single crystal diffraction, which makes it possible to decode the entire structure of the protein, but they do allow us to 'lift fingerprints' quickly and easily so that we can identify the protein and its crystal structure. This is valuable knowledge when you are working with the production of proteins."

Quick Answer

The method has great potential in the context of optimizing both quality and production processes in all production set-ups that involve solid substances. Applying the new method will make it possible to check continuously for changes in—or transformations of—different substances used in the production process.

"The advantage of our method is that it allows you to take samples directly from a production line. You then have the results within 15 minutes and can tell precisely what crystalline material is involved. In addition, the X-ray beams we use can easily be generated using standard laboratory equipment," relates Christian Grundahl Frankær. The encouraging results are only the beginning.

"What we want to do now is to test how far we can push the method. We have already established that it works on proteins, but will it also work on other complex products? And what happens if we take the samples to the synchrotron in Grenoble, where the X-ray beam is a million times more powerful than the one we have in our laboratory?" asks Christian Grundahl Frankær.

Provided by Technical University of Denmark

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