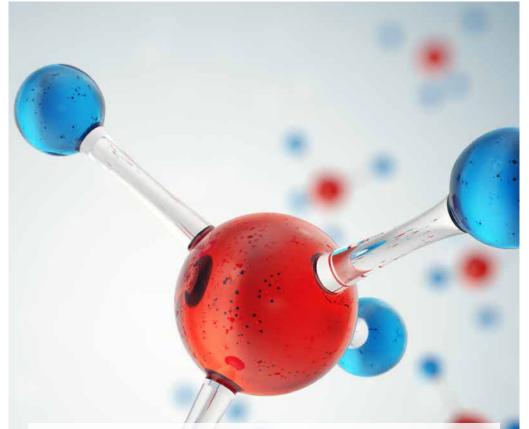
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### SHAPING THE FUTURE OF CRYSTALLOGRAPHY

Gaining momentum in science and industry, electron diffraction will help overcome existing limitations for the analysis of nano-crystalline systems

## ELDIGO-SCIENTIF



ELDICO Scientific AG (The Electron Diffraction Company) is a Swiss technology and service company that was founded in 2019. ELDICO develops, manufactures and commercializes electron diffractometers, i.e. novel analytical instruments for electron-based crystallography, enabling to investigate nano-crystalline samples.

Proof-of-concept was achieved in 2018 (ETH Zurich, C-CINA Basel) as part of a Nano-Argovia project of the Swiss Nanoscience Institute (SNI). It was published and awarded Top 5 **"Breakthrough of the Year 2018"** by the leading science magazine SCIENCE.

Since then, we have successfully built a flourishing organization. More than 20 technical experts and developers from five industrial partners, among some of the world's leading engineering companies as well as component suppliers are intensively working together to bring the first dedicated electron diffractometer to market.

ELDICO's clients are industrial and academic researchers in large and fast-growing areas such as the pharmaceutical industry, the electro-mobility and the advanced materials/ MOFs sector. The company partners with leading engineering companies and component suppliers to deliver superior performance.

**Shaping the Future of Crystallography,** for us, means supporting academic and industrial scientists in obtaining relevant structural information faster, with better quality and at lower cost.

# What the future of electron diffraction looks like



In an article on crystallography and electron diffraction[1], the innovative potential of new crystallographic methods such as electron, neutron and synchrotron radiation has clearly been recognized. These techniques are now making it possible to study atomic structures of previously inaccessible crystalline solids.

In addition to the performance of new detector systems, the benefit from increased computing power and the Cambridge Structural Database (CSD), which contains one million crystal structures allowing data to be used in ways that would have been unimaginable in the past, the article emphasizes the role of electron diffraction. Addressing the availability of sufficiently large crystals as one of the main (and best-known)) bottlenecks, the author sees electron diffraction and quantum crystallography to have enormous potential: one current development is the structure elucidation of nanocrystalline molecular compounds by electron diffraction. Thanks to a combination of a hybrid pixel detector with a transmission electron microscope, it is now possible to determine the structure of single crystals as small as a few tens of nanometres.

We believe that the need for a microED device, which is mainly an electron microscope that is very expensive (and, in our view, not very

## Voice of the Customer

suitable), will be causing the next bottleneck further down the road towards a swift and accurate analysis of nanocrystalline samples. Moreover, these experiments are not within reach for the majority of crystallographers, forcing scientists around the world to rely on data from alternative sources.

ELDICO's dedicated electron diffractometer is a highly advanced instrument concept that will enable the analysis of nano-sized solid compounds. Organic chemists will be among the first users to learn about and appreciate the advantages of this disruptive technology. We are currently in dialogue with many user groups and are finding a keen awareness of the methodology itself as well as great interest in our instrument concept, which will beat the "retrofitted" electron microscopes in terms of usability, quality, time to obtain data and – last but not least – in cost.

#### Dr. Eric Hovestreydt

Founder and CEO of ELDICO Scientific

" ... an interesting opportunity (...) for detailed 3D structure analysis on compounds presenty impossible to measure, e.g. nanosized zeolites."

Jamie Yang, Huub Kooijman and Ralph Haswell, Shell, Global Solutions International B.V., Amsterdam/NL

#### "ELDICO Scientific has found a way to address the most pressing problems of using conventional TEMs for electron crystallography."

Prof. Dr. Christian W. Lehmann, FRSC, MPI für Kohlenforschung, Mülheim an der Ruhr/DE

References:

<sup>[1]</sup> Trendbericht Analytische Chemie, Nachrichten aus der Chemie, 68, April 2020, 56-57 and references therein

### Product & technology

Electron Diffraction (ED) is gaining momentum in science and industry. The application of ED for performing nano-crystallography is a disruptive innovation that will open up fascinating new perspectives, in particular for organic compounds required in the fields of chemical, pharmaceutical and advanced materials research. Unlike transmission electron micro-scopes (TEM), the ELDICO device is dedicated solely to ED, making it possible to outperform TEM in diffraction by delivering results with better quality and greater reliability and – by making preparative chemistry (i.e. crystallization) obsolete – much faster at significantly lower investment levels.



#### The ELDICO Electron Diffractometer

Shaping the future of crystallography with better quality, faster and at lower cost: electron diffraction eliminates the crystal size problem by entering the sub-µm regime. The ELDICO Scientific Electron Diffractometer is designed to measure samples in the nanometer range of organic and inorganic compounds and is targeted to achieve in most cases a resolution of up to 0.84 Å with at least 60-70% complete datasets having a Rint of <20%. Those data typically allow for structure solution and refinement down to R1 values of <10% in 75% of cases. Unit cell determination can be accurate to 1: 1,000.

### Specifications

#### THE SYSTEM CONSISTS OF:

• An electron gun with HV supply

Source	
Emitter Acceleration	LaB <sub>6</sub> 160kV
Beam size	40 nm in imaging at sample
beam size	$0.2 - 1.0 \ \mu m$ in diffraction at sample
<ul> <li>Column with electron-optical system</li> </ul>	
Imaging	
Mode	STEM single image scanning
Field of view	0.5 mm to 0.5 µm
Dose per image	0.025 e/Ų
Resolution	20 nm
Diffraction	
Mode	continuous rotation 0.82 Å
Resolution	0.82 A
Sample handling	
Load-lock system for sample insertion	
Goniometer for sample handling	
Туре	single axis -70° - +70°
Rotation Speed	1°/s - 6°/s
Accuracy	0.01° at 1°/s
Sphere of confusion	<0.5 µm
Detection system	
Hybrid-pixel detector	
Sensor	Si
Number of pixels	512 x 512
Energy range	30 – 200 keV
Distance to sample	fixed
<ul> <li>Software package</li> </ul>	
Control of the electron source Calibration of the electron source and optics Image and diffraction modes available Crystal search and positioning at range of magnification Centering of the crystal on the goniometer axis Data collection menu Crystallographic features Data processing hkl-I file generations	
• Vacuum system	
• Electronics	
Housing	
• PC	
Requirements	
Room	laboratory with standard dimensions
Power	≤32A, 3Phase
Water	≤2 liters / min

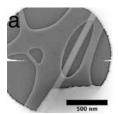
### Claims

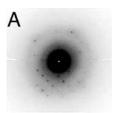
Sample size from 10 to 1000 nm Radically simplified EM design Improved goniometer R<sub>1</sub> below 10%

## Proof of concept on organic samples: new polymorph of a highly active API

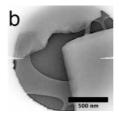
#### Experimental

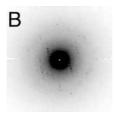
Tecnai F30 TEM at 200 kV  $\lambda$  = 0.02508 Å Dose rate of ~0.01 e-Å-<sup>2</sup>/s-1 Crystal thickness: ca. 300 nm





Sample A (confidential) Known polymorph Triclinic unit cell





Sample B (confidential) New polymorph Orthorhombic unit cell

### Key publications

Electron diffraction (ED) is gaining world-wide attention in the crystallography community and is one of the most rapidly developing and exciting fields of crystallography. Over the past two years, every relevant congress or conference dedicated to crystallography, chemistry, material sciences, geology or bio-molecules has featured the topic of ED.

The following is an overview of the most interesting and insightful scientific publications.

"Design guidelines for an electron diffractometer for structural chemistry and structural biology." T. Grüne et al., Acta Cryst., 2019, D75, 458-466.

**"Electron diffraction of submicron-sized 3D crystals."** Andreas Förster and Sacha De Carlo, IUCr Newsletter, 2019, 27, 2, 31.

#### "3D Electron Diffraction: The nano-crystallography revolution."

Mauro Gemmi, Enrico Mugnaioli, Tatiana E. Gorelik, Ute Kolb, Lukáš Palatinus, Philippe Boullay, Sven Hovmöller, and Jan Pieter Abrahams, ACS Cent Sci., 2019, 5, 8, 1315-1329.

"Rapid Structure Determination of Macrocrystalline Molecular Compounds using Electron Diffraction." *T. Gruene et al., Angew. Chem. Int. Ed., 2018, 57, 16313-16317.* 

#### "Collecting 3D electron diffraction data by the rotation method."

Daliang Zhang, Peter Oleynikov, Sven Hovmöller and Xiaodong Zou, Z. Kristallogr.- Crystalline Materials, 2010, 225, 2-3, 94–102.

"Hydrogen positions in single nanocrystals revealed by electron diffraction." L. Palatinus, P. Brázda, P. Boullay, O. Perez, M. Klementová, S. Petit, V. Eigner, M. Zaarour, S. Mintova, Science, 2017, 355, 6321, 166-169.5.

"Electron diffraction determines molecular absolute configuration in pharmaceutical nanocrystal." Petr Brázda, Lukáš Palatinus and Martin Babor, Science, 2019, 364, 6441, 667-669.

"Polymorph evolution during crystal growth studied by 3D electron diffraction." Edward T. Broadhurst, Hongyi Xu, Max T. B. Clabbers, Molly Lightowler, Fabio Nudelman, Xiaodong Zou and Simon Parsons, IUCrJ., 2020, 7, 1, 5-9.

#### "Towards quantitative treatment of electron pair distribution function."

T. E. Gorelik, R. Neder, M. W. Terban, Z. Lee, X. Mu, C. Jung, T. Jacob and U. Kaiser, Acta Cryst., 2019, 4, B75, 532-549.

### We are ELDICO Scientific

A strong team with complementary skills. Many years of experience in management, industry and the scientific field. Ideally positioned to master the diverse challenges of the new venture.



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### Scientific Advisory Board

ELDICO Scientific has appointed a first-class Scientific Advisory Board, consisting of pioneers in crystallography and electron microscopy from science and industry who will support the company in the development of its electron diffractometer.



#### Ute Kolb, PhD

Head of the Centre for High Resolution Electron Microscopy (EMC-M) Johannes Gutenberg University, Mainz, Germany Professor at the Faculty of Materials Sciences and Geo Sciences Technical University Darmstadt, Germany



Mauro Gemmi, PhD Director at the Centre for Nanotechnology Innovation@NEST of Istituto Italiano di Tecnologia, Pisa, Italy



Bernd Hinrichsen, PhD Head of the XRD, electron microscopy and NMR labs BASF AG, Ludwigshafen, Germany



Jeroen van Bokhoven, PhD Associate Professor of Heterogeneous Catalysis Department of Chemistry and Applied Biology, ETH, Zurich, Switzerland

#### INDUSTRIAL PARTNERS



#### ASSOCIATIONS



### SUPPORTING ORGANISATIONS





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