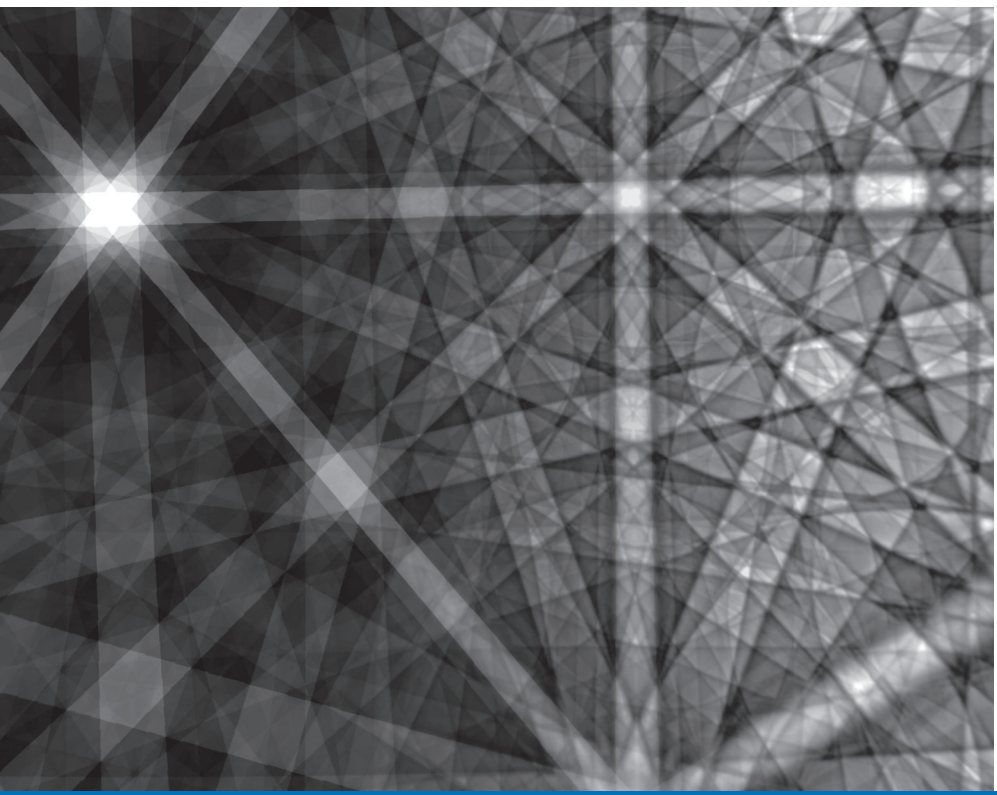
ESPRIT DynamicS

- High Resolution EBSD Pattern Simulation

EBSD

Innovation with Integrity

High Speed Realistic Pattern Simulation



ESPRIT DynamicS is a powerful and hardware-independent dynamical EBSD pattern simulation software. Using a revolutionary software engine it makes full use of available computing power to provide realistic pattern simulations within shortest times. The wealth of detail compared to common kinematic pattern simulations in combination with advanced software tools supports highest demands in EBSD pattern analysis.

Electron Backscatter Diffraction (EBSD) relies on the analysis of electron Kikuchi patterns which are obtained from microscopic regions of a sample in a scanning electron microscope. The EBSD pattern simulations provided by the ESPRIT DynamicS software greatly facilitate highly accurate analysis of crystal orientations and phases.

Main features

ESPRIT DynamicS incorporates all common simulation approaches for EBSD patterns, from simple kinematic simulations to sophisticated dynamical simulations which provide the highest level of realism.

ESPRIT DynamicS can be used for vendor-independent simulation of experimental data irrespective of the specific EBSD hardware. The software includes an automatic single-pattern calibration, with optional manual and cross-correlation-based fine-tuning.

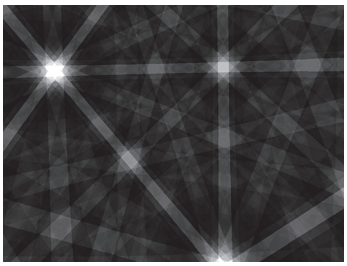
Applications at a Glance

ESPRIT DynamicS is designed to support

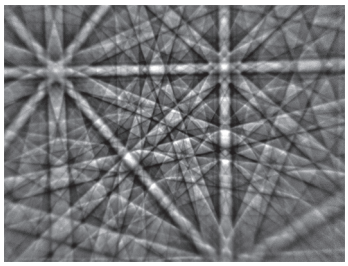
- Simulation of EBSD pattern fine structure:
  - HOLZ (Higher-Order Laue Zone) rings
  - Patterns of non-centrosysmmetric crystals (e.g. GaP)
  - Energy-dependent EBSD, i.e. changes to patterns in dependence on electron beam energy
- Highly accurate phase identification, including small particles using TKD (Transmission Kikuchi Diffraction)
- Exact orientation analysis
- System calibration (pattern center PC, sample-to-screen distance SSD)

Simulation Models and Visualization

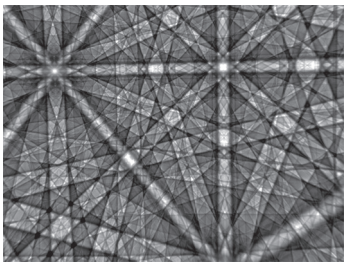
Simulation models



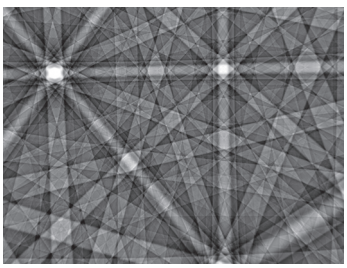
Kinematic simulation



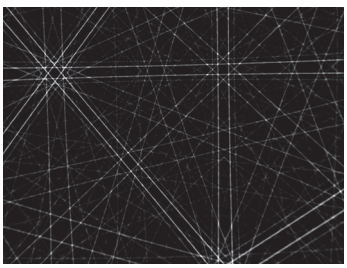
Experimental pattern



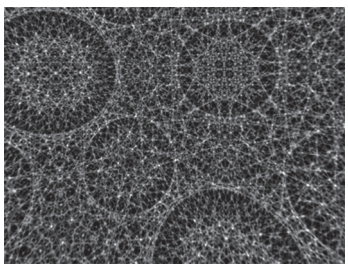
Dynamical simulation



Pseudo-dynamical simulation



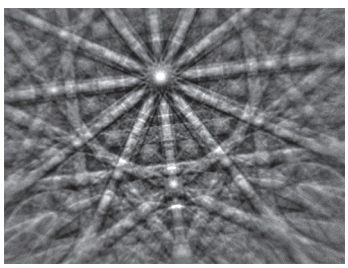
Strong Bragg reflectors used for kinematic simulation



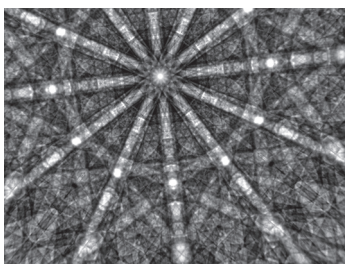
Bragg reflectors used for dynamical simulation

Available simulation models demonstrated using Austenite (Fe fcc) as an example

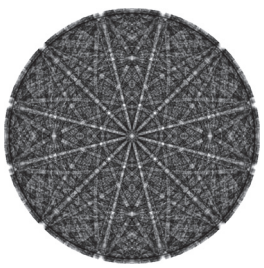
Visualization options



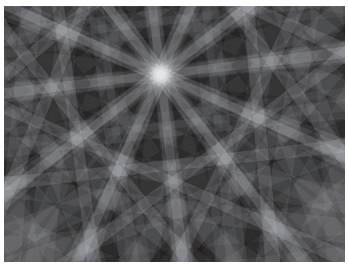
Experimental pattern



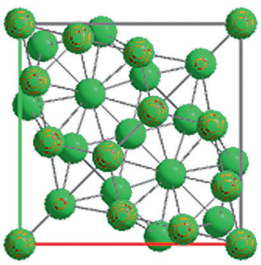
Gnomonic projection: Dynamical simulation



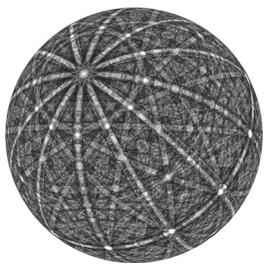
Stereographic projection



Gnomonic projection: Kinematic simulation



Crystal structure



Diffraction sphere

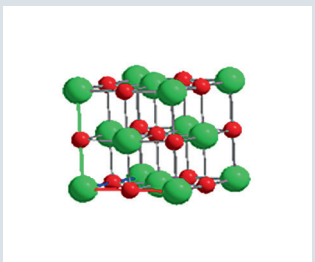
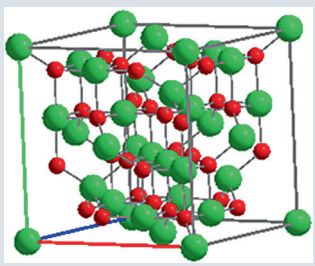
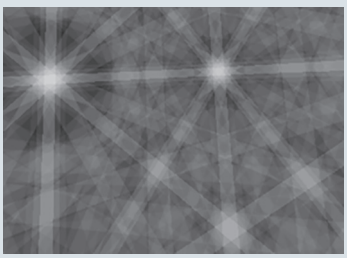
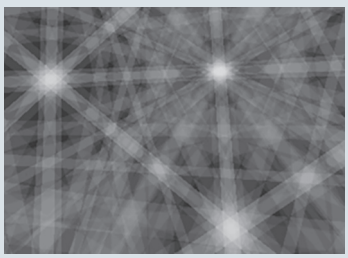
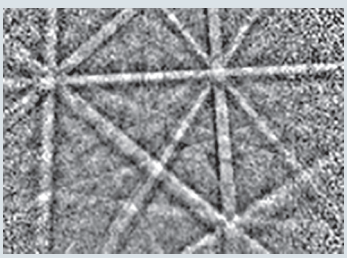
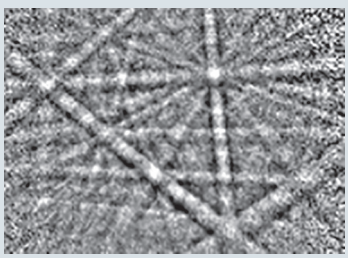
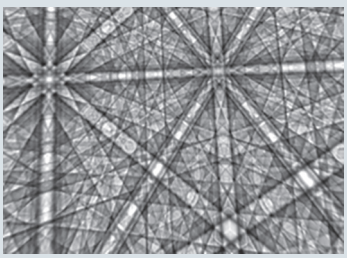
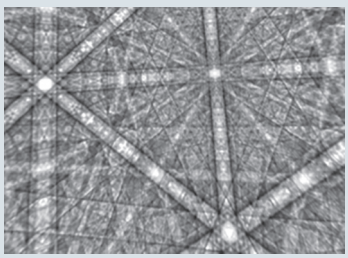
Different visualization options using the sigma-phase as an example

Application Example: Iron Oxides

Iron oxides are important compounds which are widespread in materials science (e.g. steel corrosion) and geology (e.g. ore deposits).

The crystal structures of iron oxides show many similarities, which can make them difficult to distinguish reliably, also by EDS.

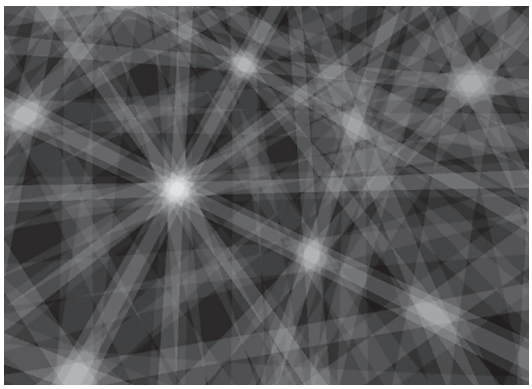
Identifying correct iron oxide phases

Wuestite	**Magnetite**	
FeO $Fm\bar{3}m$ (No. 225) cubic	Fe_3O_4 $Fd\bar{3}m$ (No. 227) cubic	Crystal structures and symmetry groups
		
		Kinematic simulations show very similar patterns
		Experimental low pixel resolution patterns (160x120) acquired at high speed (7ms), obtained with the Bruker *e⁻Flash* EBSD detector
		Dynamical simulations reliably capture the slight differences between the two oxide phases
$r_{Wuestite}$ **= 0.62** $r_{Magnetite}$ = 0.53	$r_{Wuestite}$ = 0.41 $r_{Magnetite}$ **= 0.64**	The pairwise cross-correlation coefficient **r** indicates the correct phase for each of the two experimental patterns

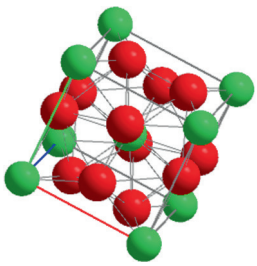
Application Example: Chromium Silicide

Ring-like features around zone axes can be very distinctive for certain phases in experimental EBSD patterns. Only the dynamical electron diffraction theory is able to provide a realistic simulation of Higher-Order Laue Zone (HOLZ) rings and other pattern fine structure. This can be useful for ultra-accurate phase verification in addition to other methods.

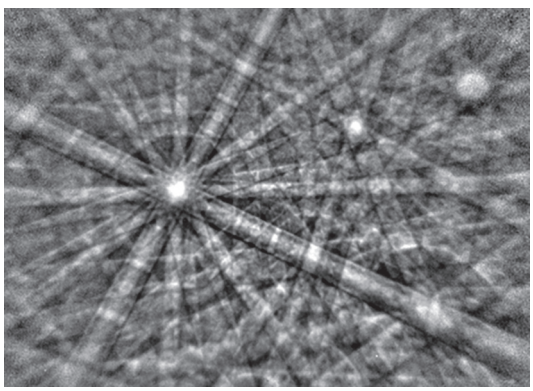
Accurate reproduction of Cr_3Si HOLZ rings



Kinematic simulation

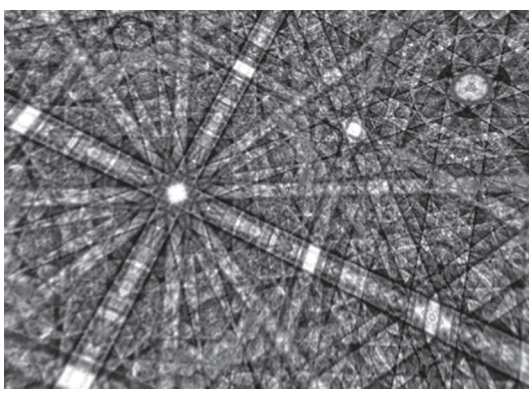


Cr_3Si crystal structure



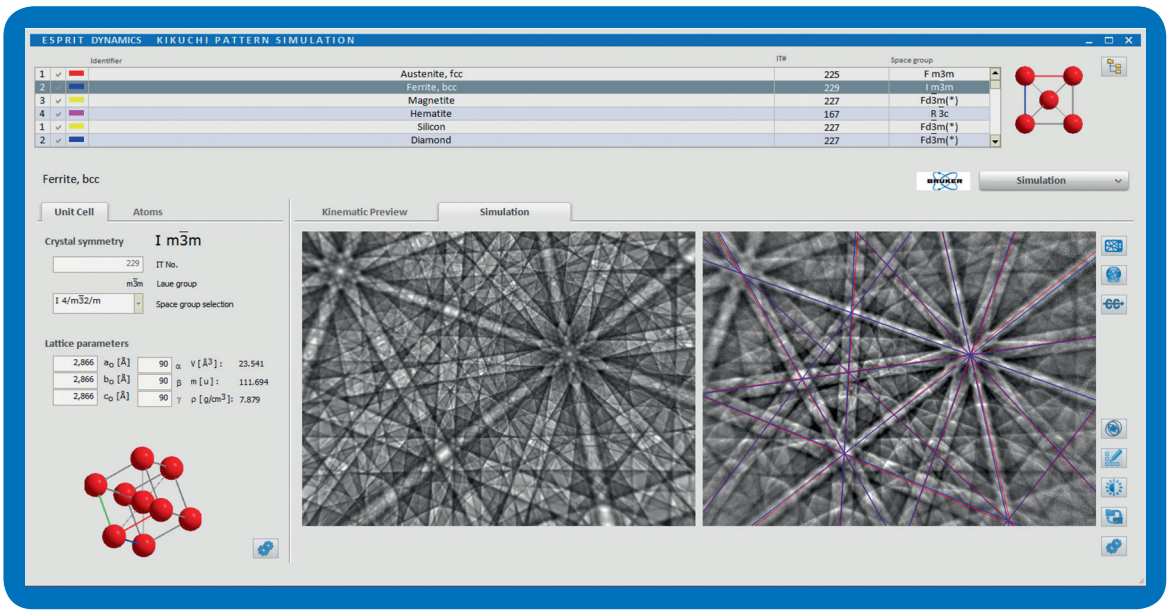
Experimental pattern

High resolution experimental Kikuchi pattern acquired using the Bruker ***e⁻Flash*** EBSD detector



Dynamical simulation

The detailed fine structure in the patterns is accurately reproduced: Characteristic HOLZ rings are found around the prominent zone axes



ESPRIT DynamicS key features

Parameter	Details
Simulation models	Dynamical, pseudo-dynamical (two-beam), kinematic box profiles, Bragg geometry
Visualization options	Projections: gnomonic, stereographic, spherical Other: experimental pattern, crystal structure, Bragg reflectors
Import file formats	Import crystallographic phase definitions in various formats, e.g. ESPRIT XML phase list files, CIF (Crystallographic Information File) CEL (PowderCell) Import single EBSD patterns in common graphics formats
Results storage and reuse	Simulate once and save master data (complete diffraction sphere) of simulation results of a specific phase for later reuse and real-time recalculation / rotation
Correlation coefficient calculation	Quantify and optimize the agreement between experimental and simulated patterns via normalized cross-correlation coefficient **r** (r=0…1; r=1 for a perfect fit; r=0 for a purely random correlation)
Crystal structure view	View crystal unit cell and change lattice parameters in a configurable display e.g. to check the influence of variation of lattice parameters on the diffraction pattern
Reflector editor	Specify which reflectors are used for the kinematical preview and for the dynamical simulations, create and modify reflector lists and parameters, select kinematically "forbidden" reflectors for dynamical simulations
Additional simulation options	Configure the (dynamical) simulation using basic (e.g. acceleration voltage, image resolution) and extended expert options

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