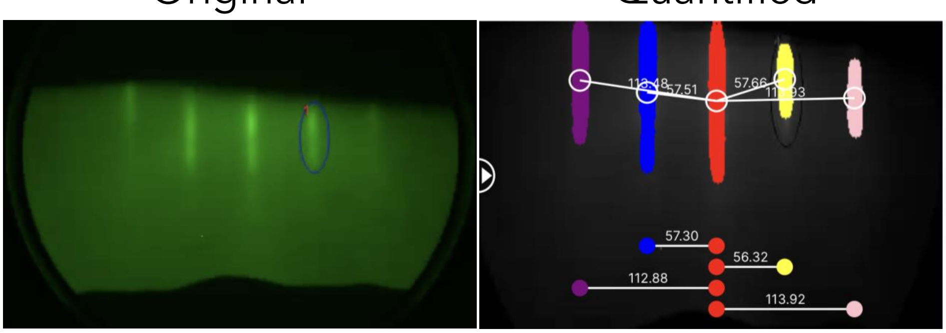
AtomCloud for MBE

Get more out of RHEED

- **Quantify RHEED patterns:** automatically generate powerful datasets.
- **Detect changes in surface lattice from RHEED videos:** automatically pinpoint when changes occurred during a process.
- **Correlate surface structure evolution with process inputs:** unify characterization with fluxes, temperature, etc. from equipment logs.
- **Develop more efficient methodologies:** save time and money using correlated RHEED as a proxy for ex-situ characterization.
- **Build a data repository:** enable large scale, fine-grained analysis of MBE processing.
- **Connect data across teams:** store, manage, and collaborate on experimental data across your entire team, maintain data continuity over time.

Original Quantified



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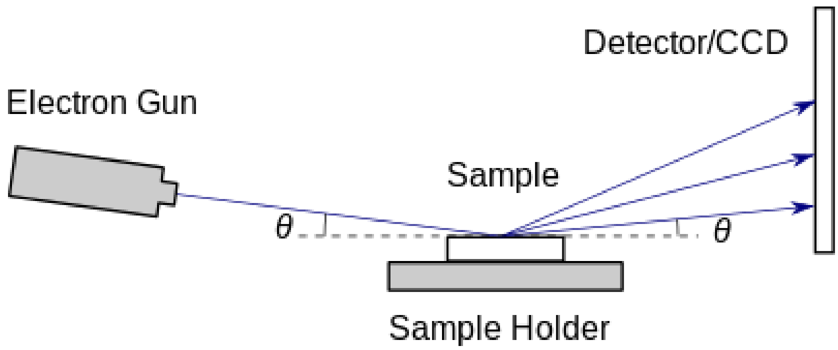
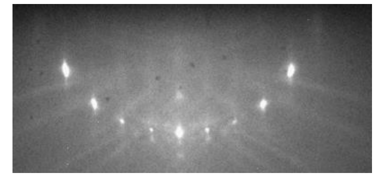
Get more out of RHEED





Reflection high energy diffraction (RHEED) provides a streaming **real-time representation of a material's surface** during processing in a vacuum chamber (e.g., growth).

The RHEED pattern contains information about:

- Surface symmetry
- Lattice spacing
- Surface morphology

Recording RHEED patterns at a single point in time (images) or as a timeseries (videos) provides a record of the state of the material in the MBE chamber.

While many RHEED features are qualitatively evident to the expert eye, **challenges in systematically extracting features from images and videos block the full potential of RHEED** from being accessible to practitioners in the daily synthesis workflow.

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Additional resources

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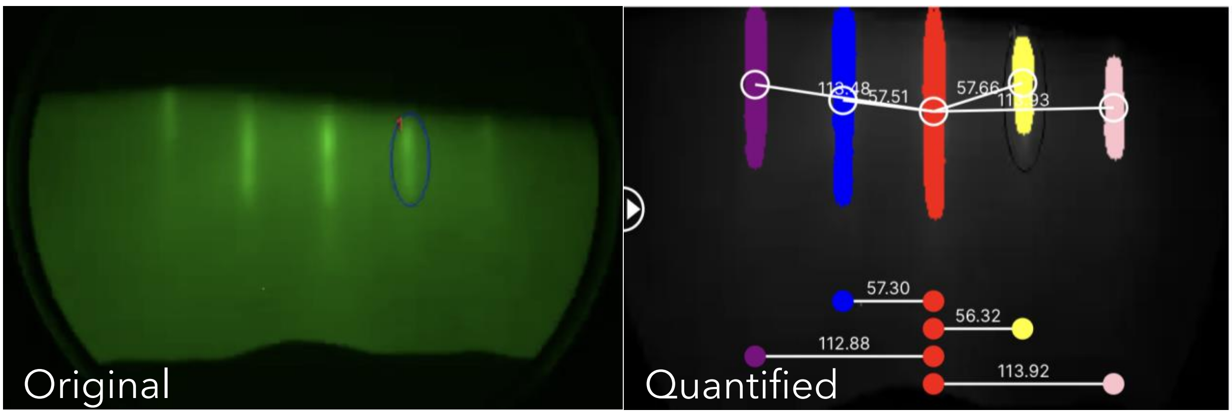
Get more out of RHEED

Each RHEED pattern can be **quantified** using a network representation (right panel) that holds information about the relative position, shape, and intensity of scattering features, providing a **fingerprint** of the material at that point in time.



AtomCloud quantifies the position of scattering features and their properties (shape and intensity)

Faint scattering features are detected without introducing operator bias.

Lattice spacing at the surface can be calculated using a pixels to Angstroms conversion (specific to the RHEED detector setup, which can be determined from the substrate).

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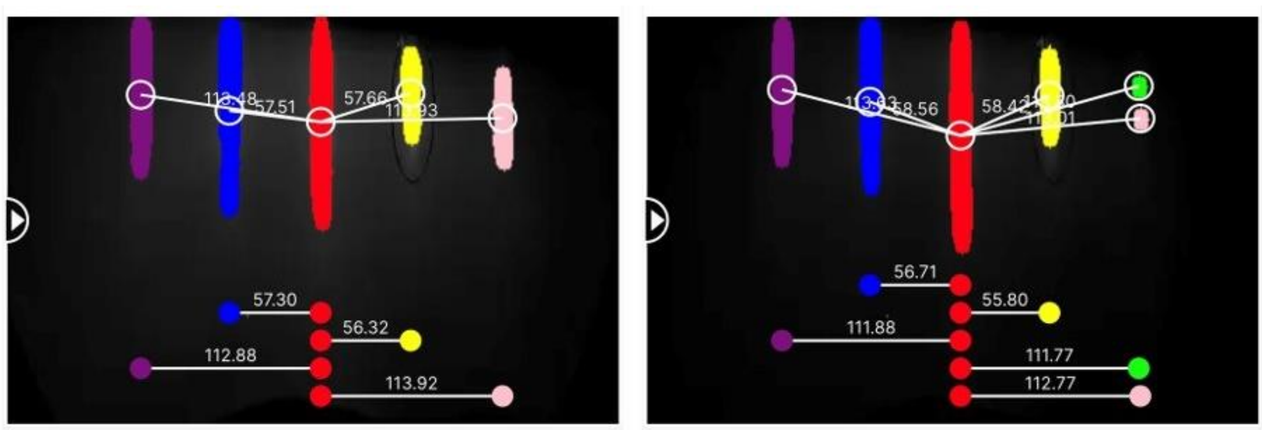
Get more out of RHEED

Fingerprints from two different images containing RHEED patterns can be extracted and **compared** qualitatively and quantitatively, providing insight into the differences in the underlying material structure.



When comparing the lattice spacing between RHEED patterns from two related samples, conclusions can be drawn about the strain state of the material.

Comparing the shape and intensity of the diffraction features from two related samples gives insight into the characteristics and distribution of the grains in the sample.

- Extent of streaks → surface uniformity
- Sharpness of streaks → uniformity of grain orientation

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Additional resources

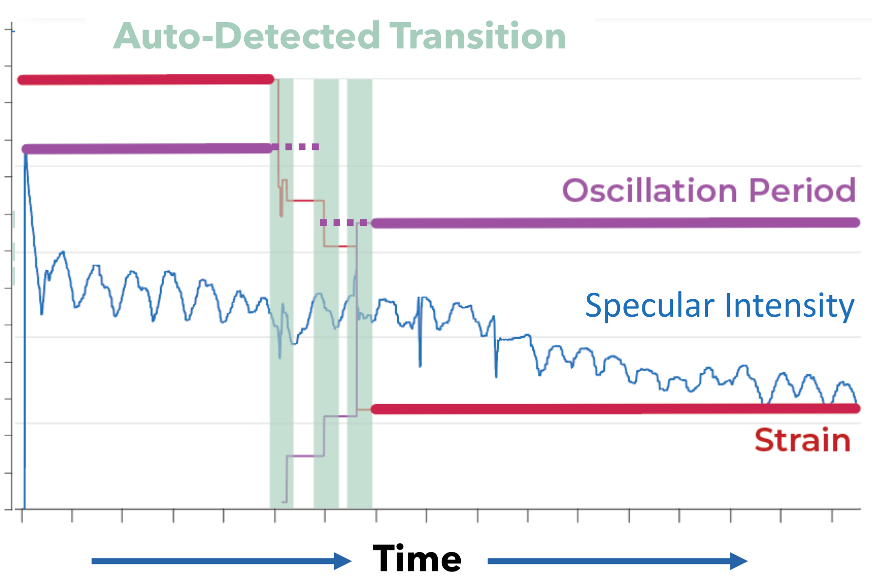
AtomCloud for MBE

Get more out of RHEED

RHEED videos contain many patterns with significant contextual relationships, providing a **surface-state-timeseries** of the recorded materials processing – de-gassing, deposition, annealing.

Comparison between video frames provides information about:
- Reconstructions (surface symmetry change)
- Strain (lattice spacing change)
- Thickness (deposition rate / rate change)
- Sample quality (morphology change)

By automating comparisons, we can extract timeseries of material characteristics and detect transitions over the course of materials processing, replacing the tedious work of analyzing each consecutive RHEED pattern manually.



Oxide heterostructure evolves -1.4% **strain** in top layer relative to bottom layer, **growth rate** accelerates in second deposition.

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[Additional resources]

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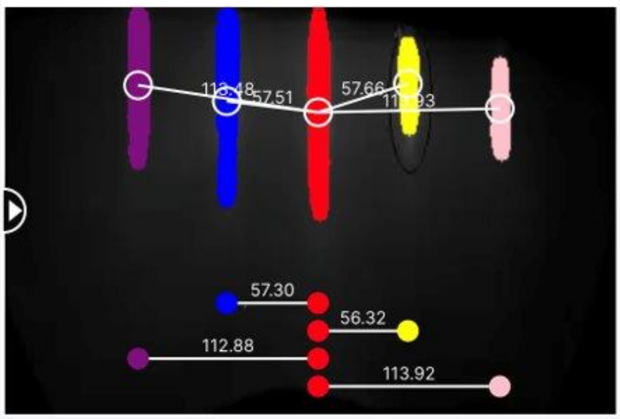
Get more out of RHEED

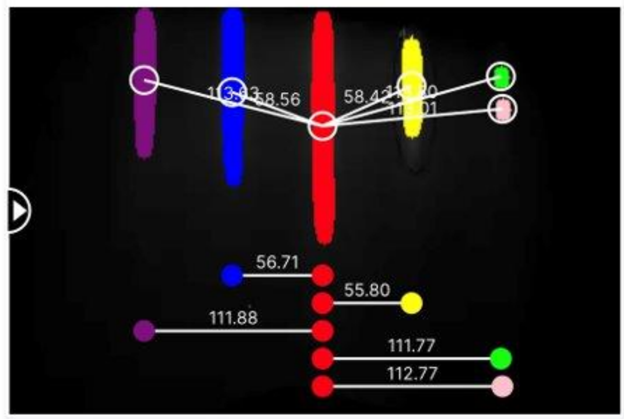
After automatically detecting transitions in a RHEED timeseries (when a change occurred) a **RHEED fingerprint comparison reveals what changed**.

Before Transition



METRIC	VALUE
Strain	-0.00951
Oscillation Period (s)	43

After Transition



METRIC	VALUE
Strain	-0.0192
Oscillation Period (s)	133

These fingerprints show an **introduction of strain** and a change in **specular oscillation period** at the transition point.

Patterns from the timeseries before and after the transition can also be examined for more details.

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Additional resources

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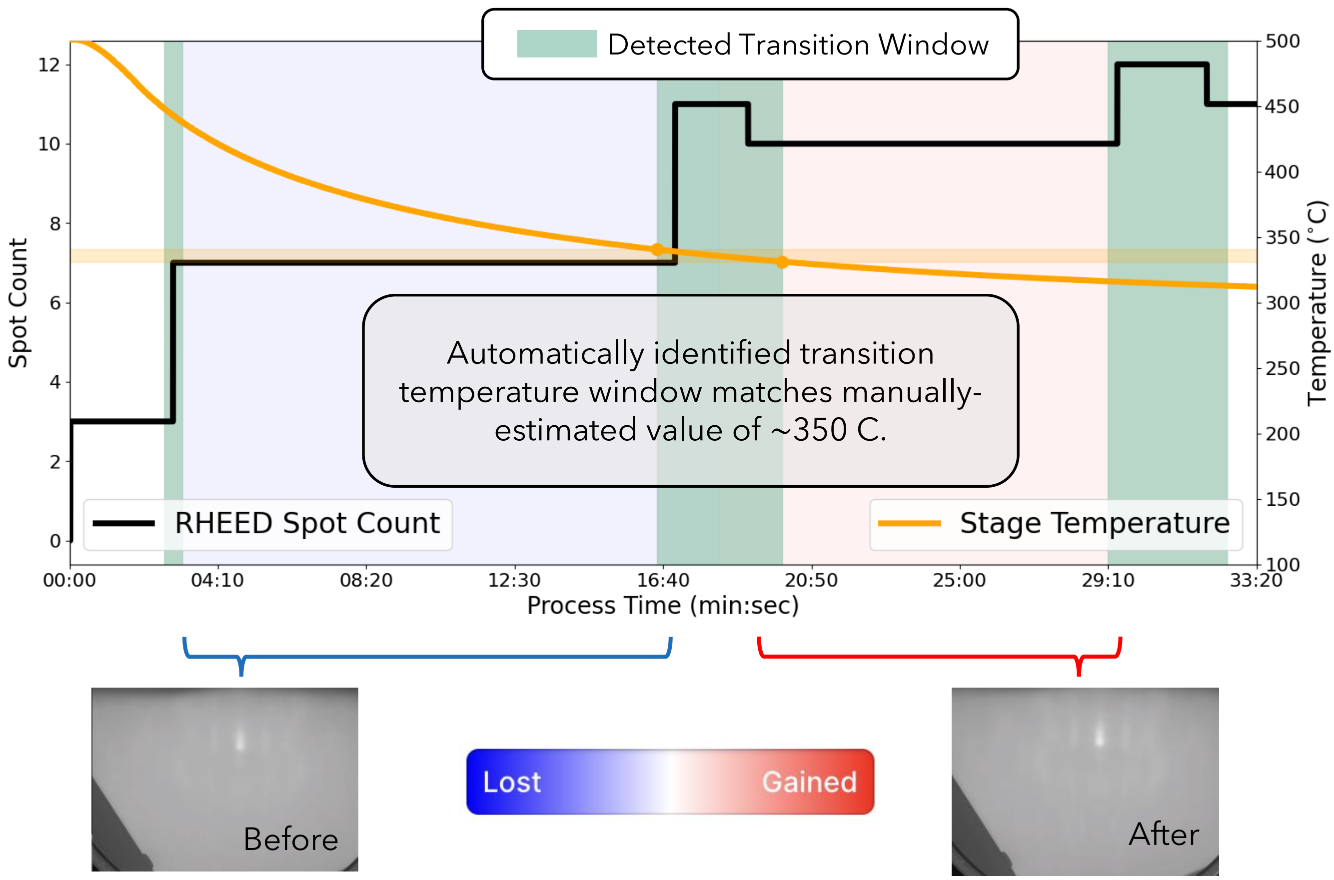
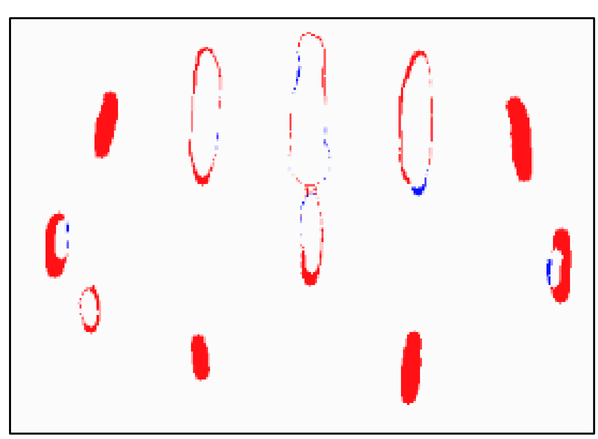
Get more out of RHEED

Timeseries of RHEED **fingerprints** can be **correlated** with materials **processing** variables like temperature, illustrating the relationship between surface structure and process inputs.



AtomCloud Pattern Differencing automatically highlights scattering gained and lost at the transition point – in this example, a new phase emerges.



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Additional resources

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Get more out of RHEED

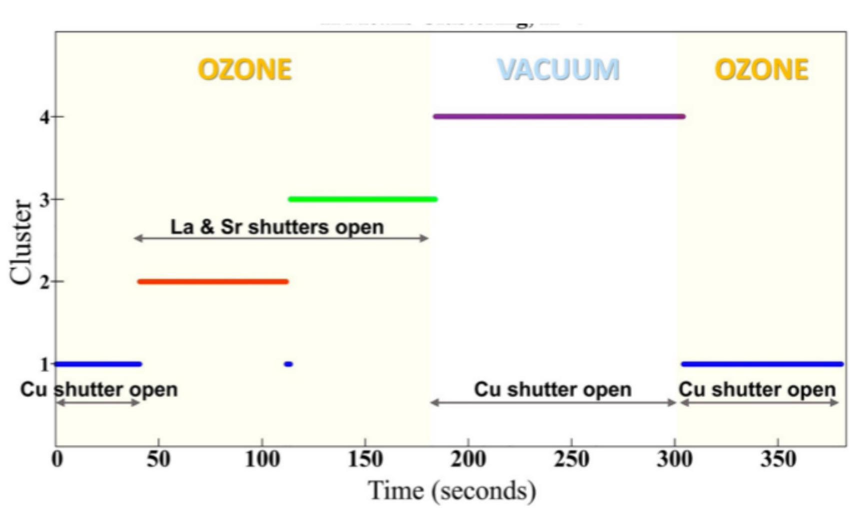
State-of-the-art: Correlating RHEED transitions and MBE inputs is a highly promising strategy for synthesis engineering that reveals the relationships between processing and surface structure.

This study uses detected RHEED transitions and process input correlations to help identify that a CuO_2 surface deposited in vacuum changes from a 4a reconstruction to a 5a reconstruction when Ozone is introduced.

Engineering ordered arrangements of oxygen vacancies at the surface of superconducting La_2CuO_4 thin films

Journal of Vacuum Science & Technology A **40**, 013214 (2022); https://doi.org/10.1116/6.0001473

Y. Eren Suyolcu[1,2,a)], Georg Christiani[2], Patrick T. Gemperline[3], Sydney R. Provence[3], Annette Bussmann-Holder[2], Ryan B. Comes[3], Peter A. van Aken[2], *and* Gennady Logvenov[2,a)]



[Link to study]

AtomCloud brings this analysis to you hands-free.

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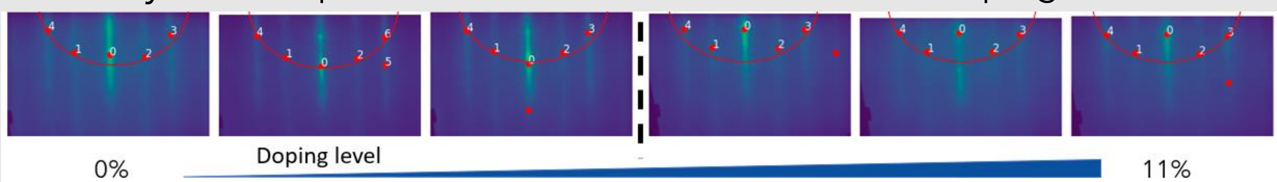
[Additional resources]

AtomCloud for MBE

Get more out of RHEED

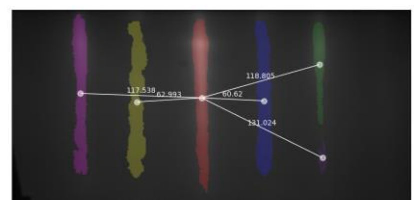
Correlate quantified RHEED patterns with ex-situ characterization—Ex: **doping concentration from XPS**

Intensity maxima position observed to correlates with doping in this case

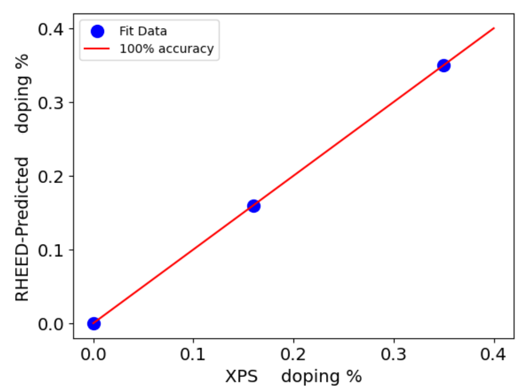


Steps:

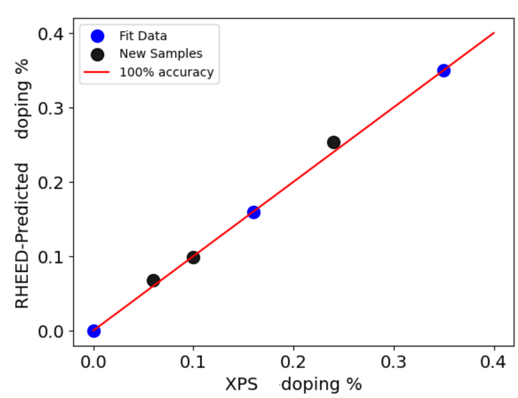
1.) Run automated feature extraction on RHEED patterns (30 seconds)



2.) Take top 3 features correlated with doping-composition from XPS and fit a linear regression.



3.) Predict ex-situ characteristics (e.g., doping-composition) for subsequent samples



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AtomCloud FAQ

What do I need to change about my hardware setup?

Nothing – **AtomCloud works with RHEED data as-collected.** Use your existing hardware and RHEED collection software, and simply export or screenshot your RHEED patterns in a common image or video format.

How do I use AtomCloud?

Take RHEED during sample preparation.

Drag and drop to the **AtomCloud** website.

Results available in **seconds** (images) to **minutes** (videos).

View and compare quantified **RHEED fingerprints.**

Export datasets and build **structure - property correlations.**

Design the next synthesis; use prior examples on **AtomCloud** as a reference.

What happens to my data behind the scenes?

The RHEED analysis pipeline is built from combinations of state-of-the-art machine learning and data analysis techniques developed and published in peer-reviewed journals for RHEED data - packaged, hosted, automated, and maintained by Atomic Data Sciences. Documentation about the data analysis is [available here].

Can I use RHEED collected from rotating sample stages?

Yes – **AtomCloud** is built to automatically process RHEED data taken from stationary and rotating stages. The data processing separates out rotational changes when identifying transitions and identifies patterns from symmetrically equivalent scattering angles to perform fingerprint analysis.

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AtomCloud FAQ

Who can see my data and analysis results?

By default, **data that you upload to the AtomCloud platform is private**, viewable only by the uploader and their organization. Intellectual property and all commercial rights for data marked as private belongs to the organization associated with the uploader, at the time of upload. Atomic Data Sciences never claims any intellectual property rights over the raw data or analysis results.

Data sharing within the AtomCloud userbase can be enabled for individual data items or for entire user accounts by marking items as shared; this will allow other AtomCloud users to view (but not edit) these data items and results.

Under private data sharing, Atomic Data Sciences reserves the right to view and use data uploaded to the platform solely for product improvements and model development. This can be changed by setting the sharing level to incognito. Data marked as incognito will be visible only to the uploading organization and excluded from Atomic Data Sciences' internal research and development.

Are there any limitations to how much data I can process?

Each data stream subscription has an annual processing credit quota which is tracked automatically in the platform. Quotas are tracked at the organizational level. Credit utilization ties back to the underlying processing and resource intensity of a particular service and different datatypes consume credits differently; for example, a quota of 1000 credits annually is roughly equivalent to 400 hours of RHEED video data at 10fps and industry standard resolution.

What happens to my data if I want to cancel my subscription?

If you decide to cancel your subscription, **you will have the option to get a copy of all data uploaded by your organization and associated results transferred to you. Data that is marked incognito or private will be removed completely from the platform**, except for a backup that Atomic Data Sciences will retain off-platform for one year beyond the cancelation date in case account restoration is requested. Data that is marked as shared will be retained on the platform.

We'd love to hear from you!

Contact us: info@atomicdatasciences.com with feedback and questions; scan the QR code on this page to learn more.

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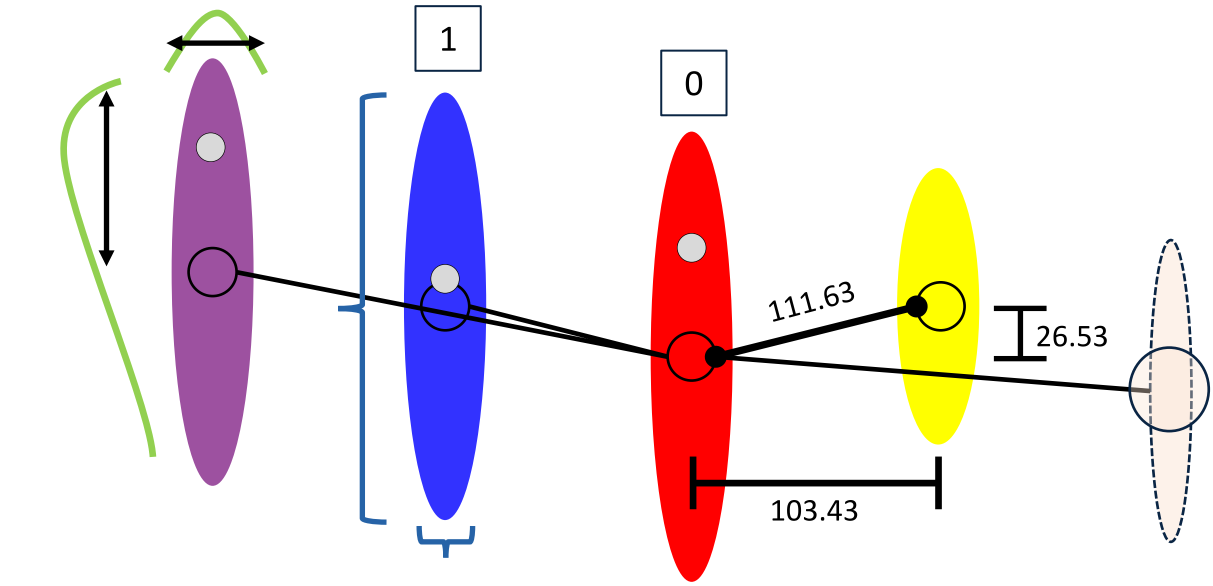
Additional resources

Anatomy of a RHEED Fingerprint



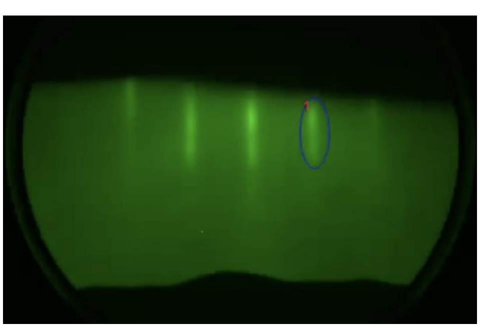
Node

- Geometric center
- Intensity maxima location
- Eccentricity; major/minor axes
- Area, streak/spot composition
- Full-width half maximum

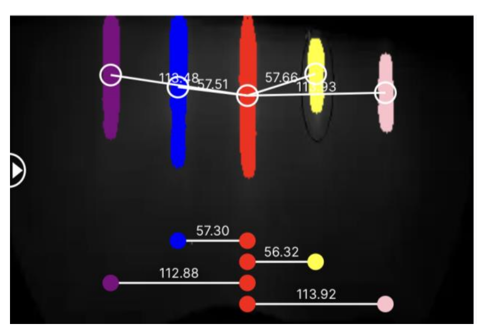
Edge

- ID Start and end node
- Total length
- Horizontal and vertical length
- Overlap

Original Image



Fingerprint Overlaid



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Additional resources

AtomCloud for MBE

Results

Single pattern fingerprints – quantify presence, position, shape, and intensity of scattering features.

Pattern comparison - extract metrics such as strain and visually represent scattering changes (loss/gain)

Timeseries analysis – identify material transitions and view growth rate and strain before and after transition points.

Processing correlation – compare surface evolution from timeseries metrics with process variables from equipment logs.

Features

Easy file upload across common image and video formats.

Automated analysis – no user inputs required to extract results.

Standardization – all data is analyzed consistently.

Stage rotation – handled automatically.

Customizable visualizations – align and compare analyses from multiple data items

Data and result access – download and programmatic interfaces.

Team oriented – share data across your lab or organization.

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Additional resources