

Digitalization of Glass Development

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⁹ GTT Technologies

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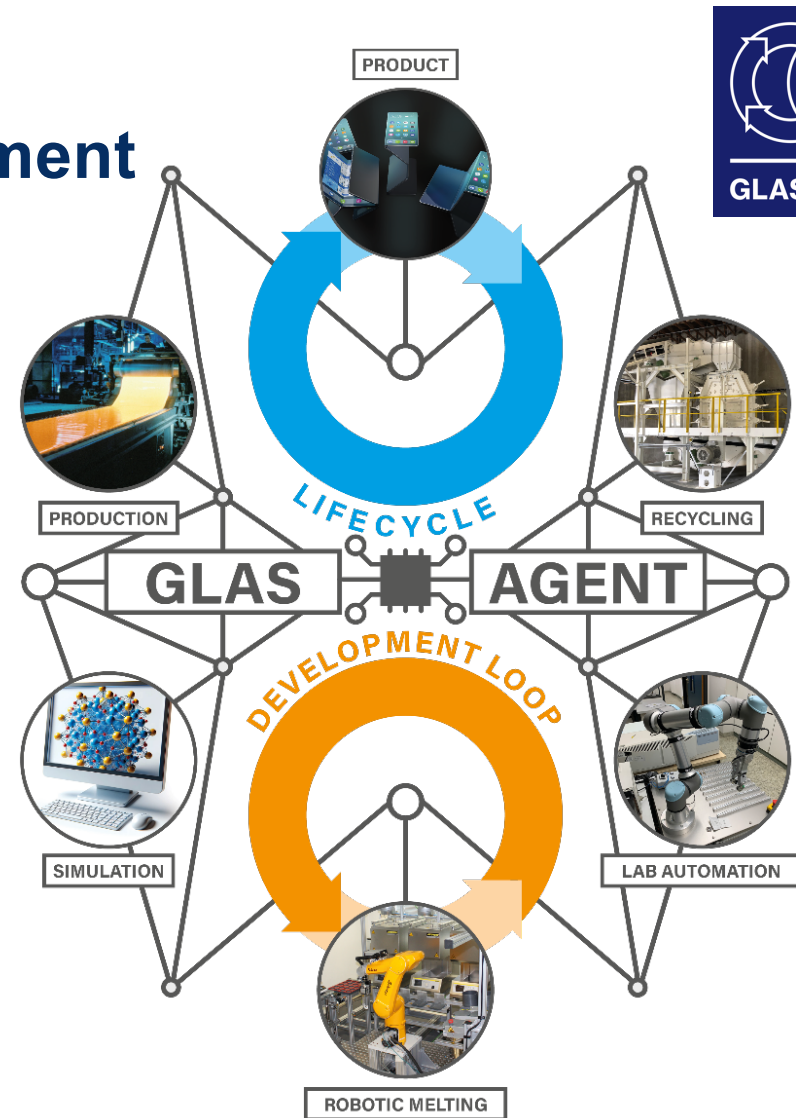
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MATERIALDIGITAL



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glass made of ideas

Pioneering the impossible since 1884

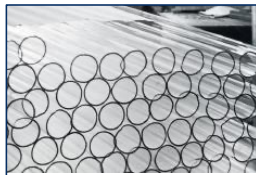


1884

Optical
glass



The most precise
microscopes



1911

FIOLAX® Borosilicate
glass tubing



Highest quality for
pharmaceutical packaging



1968

ZERODUR®
Glass-ceramic



The world's largest
telescopes



2013

SCHOTT UTG®
ultra-thin glass



Guinness World Record
– thinnest glass on earth

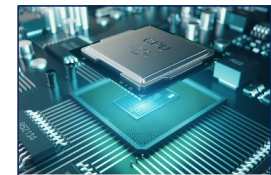


2018

High-index glass
wafers & waveguides



Fully immersive mixed
& augmented reality

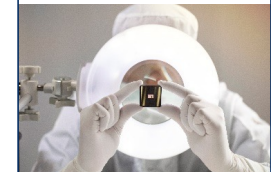


2024

Glass for advanced
chip packaging



Transforming next-gen
semiconductors



Vision for Specialty Glass Development and Life Cycle

Application determines target glass properties

Glass Development Loop

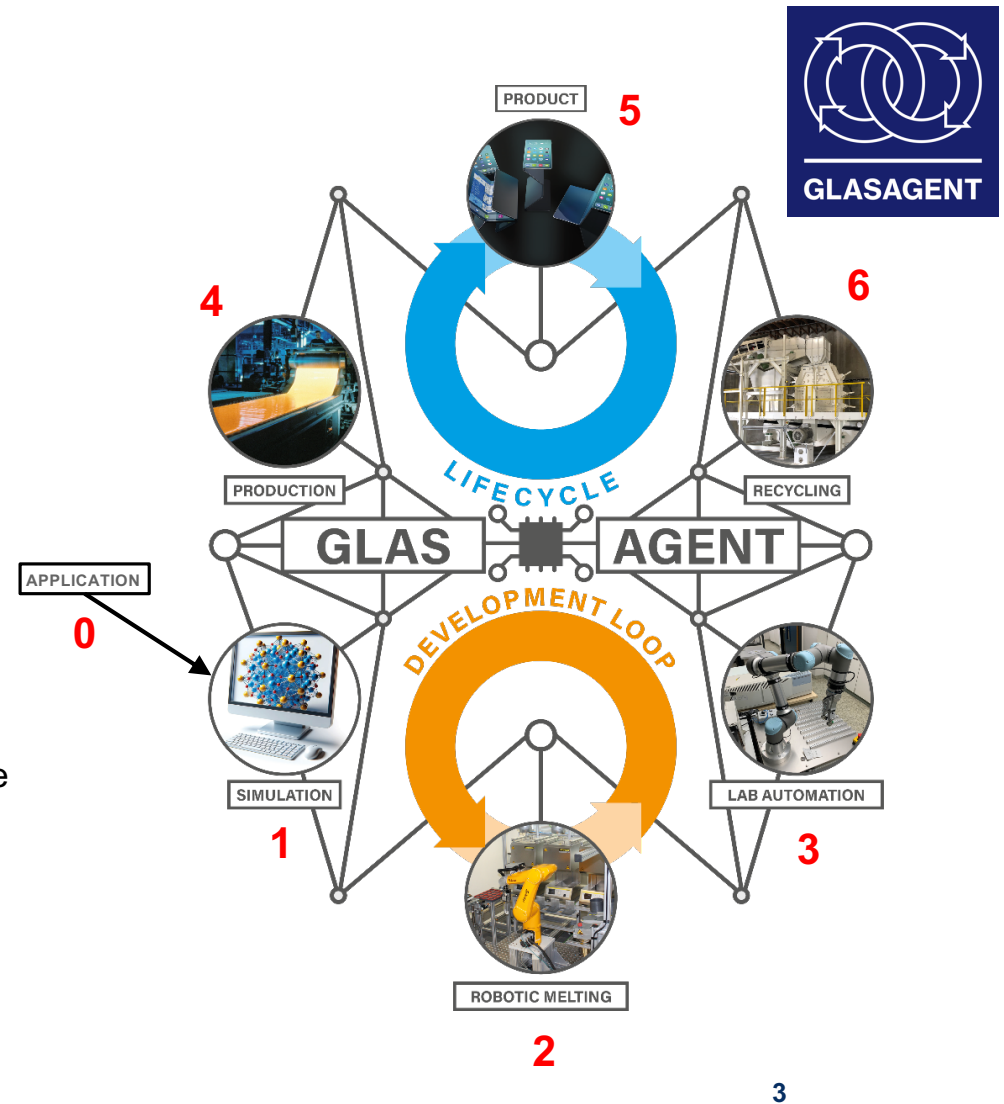
1. **Simulation** of glass properties & process (digital twin)
2. **Robotic Melt** for automated synthesis in the lab
3. **Lab automation** for automated sample analysis

Product Life Cycle

4. **Production** using recycled components and process parameters informed by digital twin
5. **Product use** without compromises in safety & performance
6. **Recycling** with separation of different special glass types

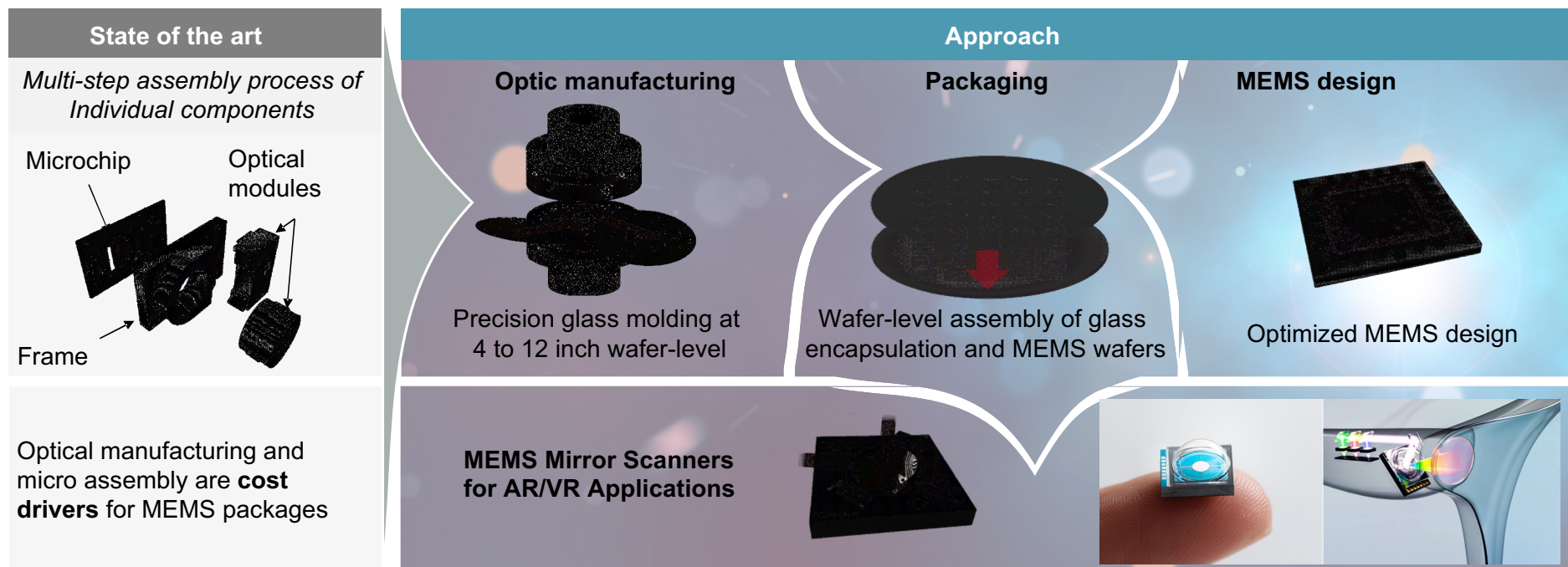
Spider in the Web

GlasAgent: Software agent integrating these loops



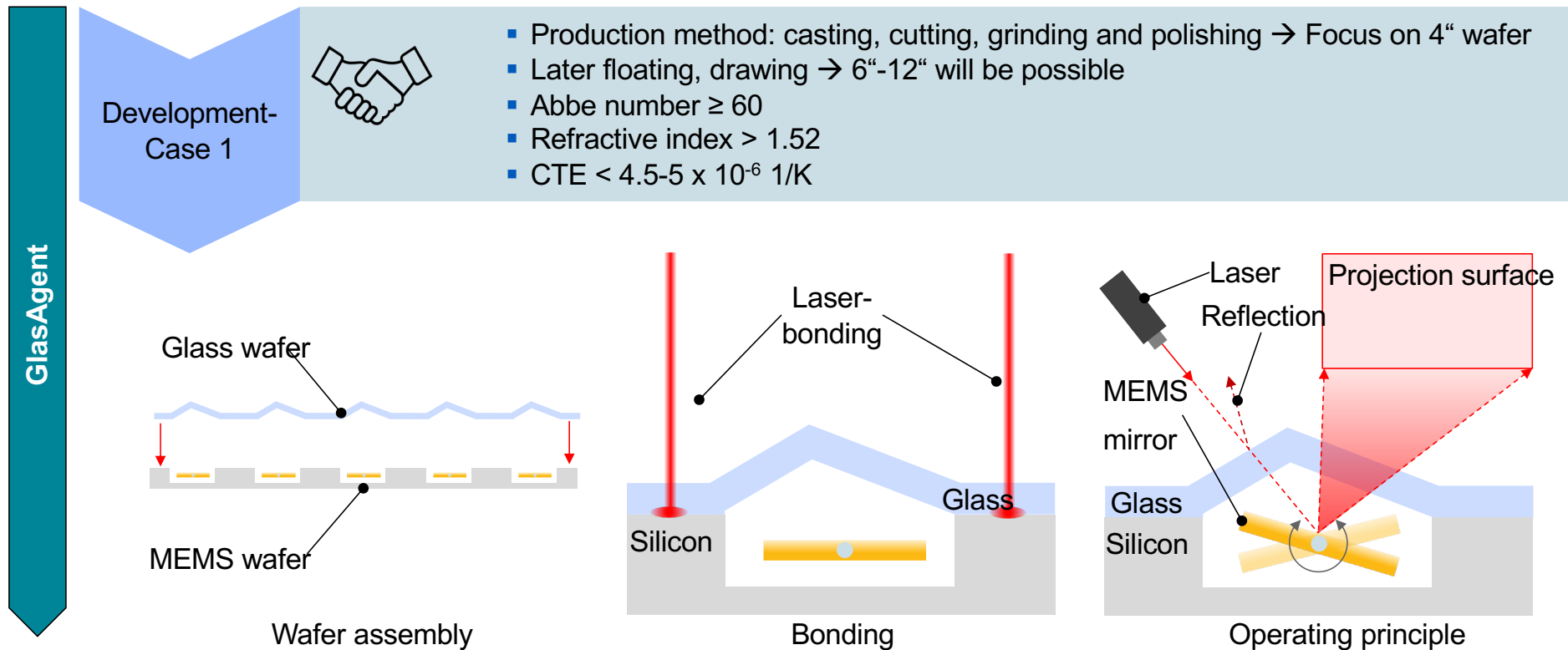
Application

New special glass for cost-effective optoelectronic components by wafer-level precision glass molding



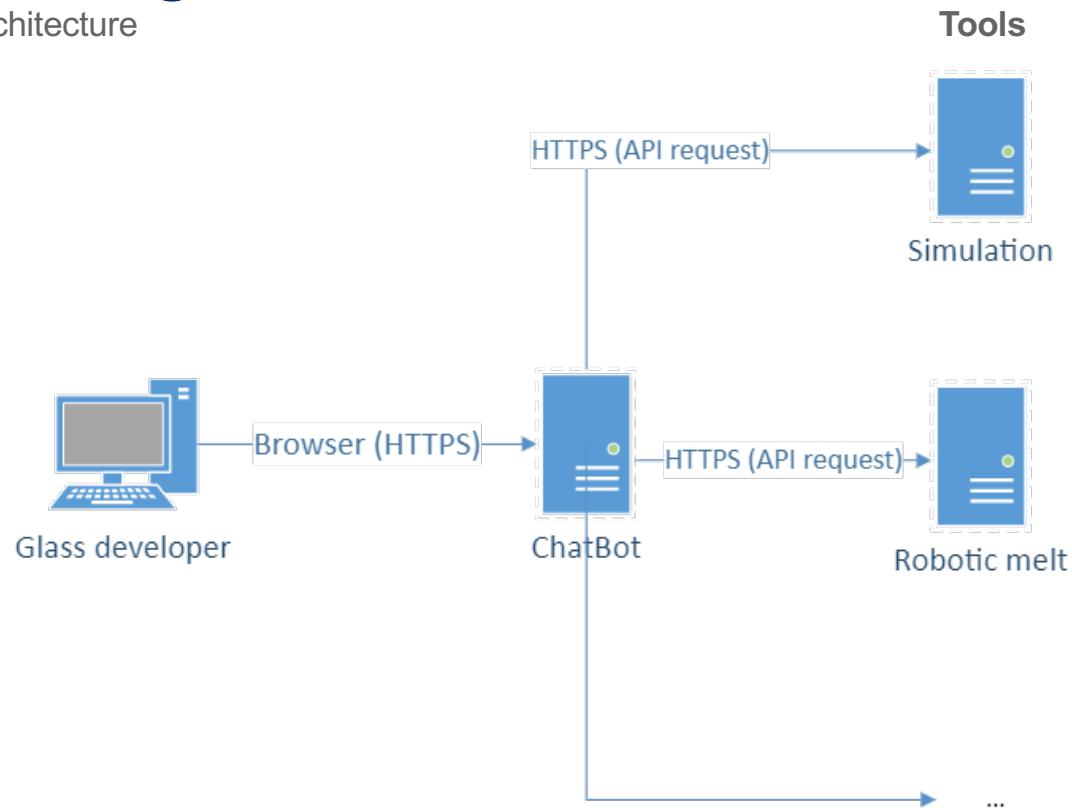
Application

New specialty glass for cost-effective optoelectronic components: optocaps for projector MEMS



GlasAgent

Architecture



FRIEDRICH-SCHILLER-
UNIVERSITÄT
JENA

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Tools

- Databases (glass properties, patents, ...)
- Models that predict glass properties based on composition
- Thermodynamic simulations via GTT
- Atomistic simulations via pyiron workflows
- Melt request for robotic melts
- ...

Ontology

- Starting from GlasDigital ontology (MaterialDigital 1)
- Include relevant ISO and DIN standards for raw materials, processing, analysis & recycling
- Integrate description of simulation methods for digital twin

GlasAgent

Chat Mockup

Glass Developer

Hello Otto, I'm looking for a glass with refractive index $> A$,
Abbe number $> B$, and CTE $< C$ ppm/K.

▶ Otto searches the internal Schott database.

▶ Otto searches external glass database.

Otto

Unfortunately, I couldn't find any known glass with those
properties. Should we try inverse design?

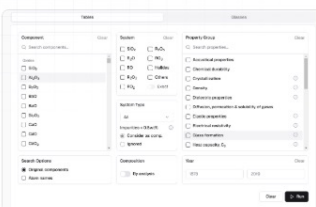
Glass Developer

Yes, let's give that a try.

Demo – SciGlass Next Search

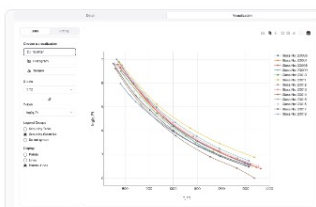
SciGlass Next

- SciGlass: Open glass property database
- SciGlass Next: web interface based on SciGlass
- Add SciGlass Next MCP endpoint to your chatbot of choice!
 - Visual Studio Code
 - ChatGPT Plus (Developer Mode)
 - Claude
 - ...



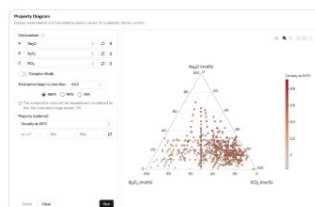
Search Panels

Search for 422K+ glasses and melts. Sourced from 40K+ literature sources.



Data Visualization

Interactive scatter plots, histograms, and ternary diagrams powered by Plotly.



Property Diagram

Display experimental property values for selected system in ternary diagram.

Data Tables

Browse and filter the glass compositions and properties powered by DataTables.

Calculation Result

Predict the properties of glass compositions with different models.

More Features Coming soon

Stay tuned for more features like commercial glass search and full-text search.

Optical Spectra

More than 15,000 optical spectra (from UV to near IR) for glasses and melts.

Glass Formation

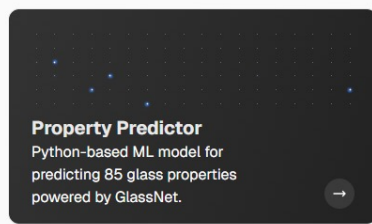
More than 4,000 ternary diagrams of glass formation.

Author Index

Easily browse and view publications by author name.

Subject Index

Specially organized topics for locating difficult-to-find database entries.



Property Predictor

Python-based ML model for predicting 85 glass properties powered by GlassNet.

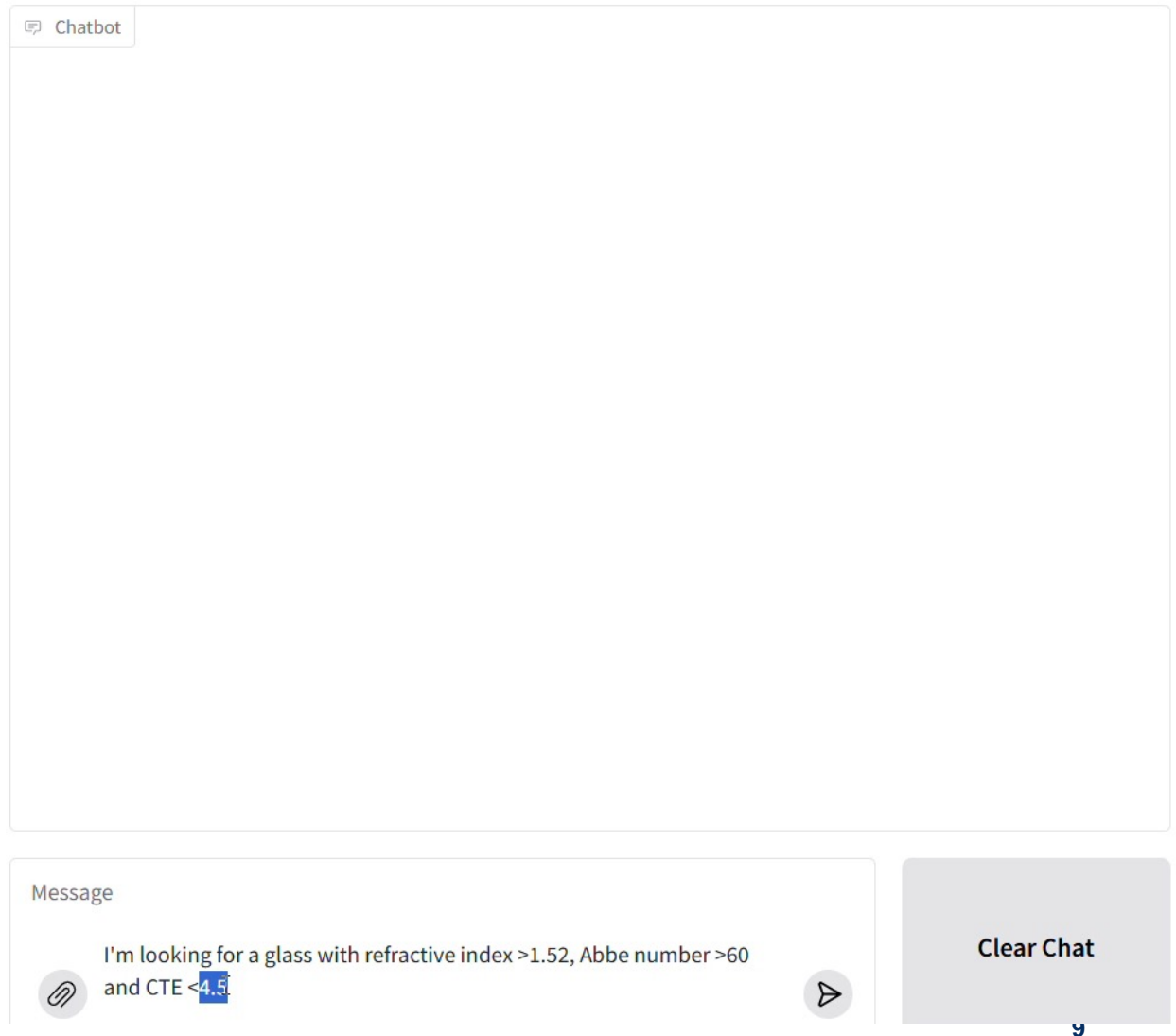
Register for free at sciglass.uni-jena.de

Demo – SciGlass Next Search

SciGlass Next

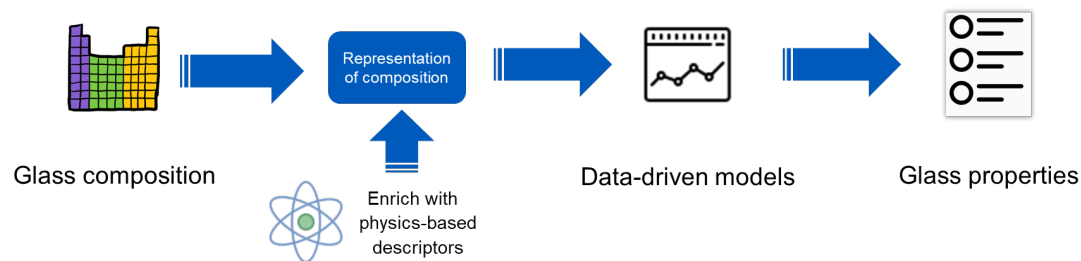
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- SciGlass Next: web interface based on SciGlass
- Register for free at sciglass.uni-jena.de
- Add SciGlass Next MCP endpoint to your chatbot of choice!
 - Visual Studio Code
 - ChatGPT Plus (Developer Mode)
 - Claude
 - ...
 - See SciGlass Next documentation

MaterialDigital 3, Project GlasAgent



1. Simulation

1.1 Data-driven models



- Given **composition** (75% SiO₂, 15% Na₂O, 10% CaO) predict **glass properties** (glass transition temperature, ...).
- Semi-empirical and machine-learning models
- Development focus:
 - Uncertainty prediction
 - Inverse design: from property to composition

Chat Mockup

Otto
Which material model should we use:

1. FancyML
2. SimpleML

Glass Developer
Please use the FancyML model.

Otto
All right. That will take a few minutes...

►Otto uses the FancyML model for inverse calculation. Progress [----]

Otto
I've determined a glass composition [XYZ], with n=1.8, Abbe number 65, and CTE 4 ppm/K, but with a low confidence score. Warning: Experimental data in this property range appears to be insufficient.

Glass Developer
That's not a bad start. What's the prediction if I increase component X by 1% and omit expensive components?

►Otto uses the FancyML model for prediction

Demo – SciGlass Next Prediction

SciGlass Next

- Using GlassNet model by D. Cassar et al.



MaterialDigital 3, Project GlasAgent

Chatbot

- CTE = 3.9 ppm/K ($39 \times 10^{-7} \text{ K}^{-1}$)
- Composition (mol%): P_2O_5 53.09, SiO_2 29.51, Al_2O_3 17.39

This glass has the **highest Abbe number** and a **low CTE**, though its refractive index is only slightly above your threshold.


If you want a higher refractive index while keeping Abbe > 60 and CTE low, the best compromise is:


Glass No. 192520 / 192529 (2000)

- $n_d = 1.549$
- Abbe number = 65.51
- CTE = 4.49 ppm/K ($44.9 \times 10^{-7} \text{ K}^{-1}$)
- Composition (mol%): CaO 4.36, MgO 15.15, Na_2O 2.96, SiO_2 71.04, ZrO_2 5.9, Al_2O_3 0.6

Do you want me to **optimize for the absolute highest Abbe number** or for a **balanced high n_d and low CTE**?

Message

 How do the properties of the last glass compare against ML predictions?

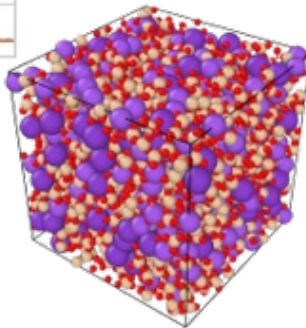
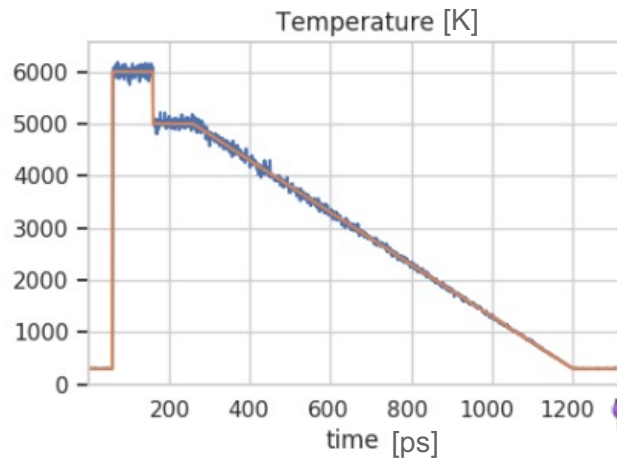


Clear Chat

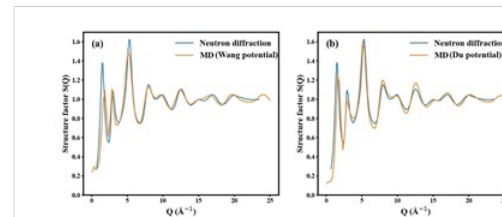
1. Simulation

1.2 Atomistic simulations

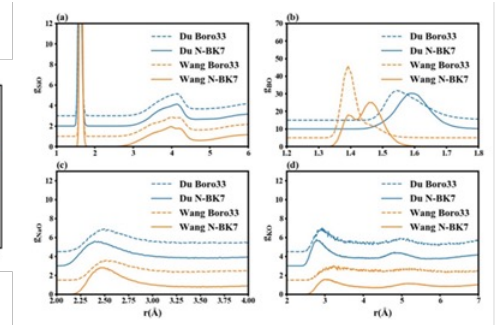
Glass structure from melt-quench procedure



→ Properties



Structure factors



Radial distribution functions

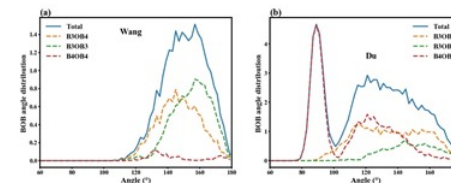


Table 2 Density of the glass samples

Condition	Boro-33	N-BK7
Experiment	2.23	2.51
Wang	2.35±0.06 (+5 %)	2.51±0.01 (+0%)
Du	2.3±0.01 (+3.14 %)	2.48±0.01 (-0.8 %)

Densities

Table 4 Elastic properties

Condition	Young's modulus (GPa)	Bulk modulus (GPa)	Shear modulus (GPa)	Poisson's ratio
Boro-33 (Experiment)	84	35.5	26.5	0.2
Boro-33 (Du, NVT)	85.8±2.7 (+3.4%)	33.3±3.3 (-6.5%)	35.1±1.1 (+32%)	0.22±0.02 (+10%)
Boro-33	51.9±3.4	29.1±1.2	21.6±1.7	0.202±0.02

Elastic constants

1. Simulation

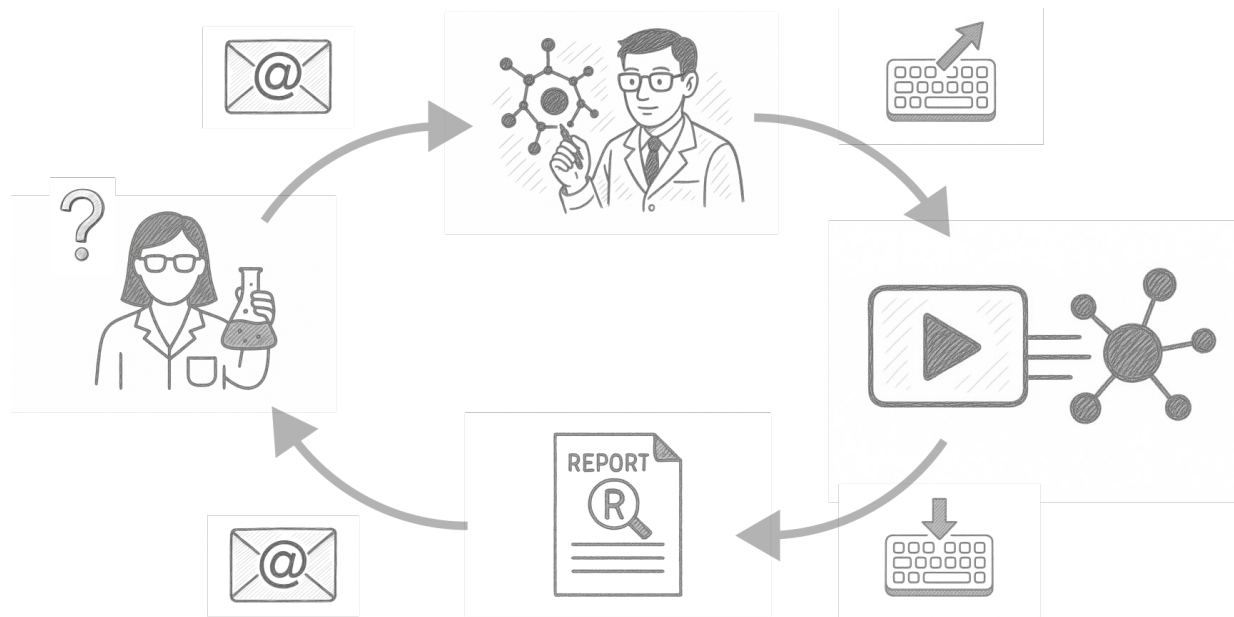
1.2 Atomistic simulations



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glass made of ideas

Typical workflow today

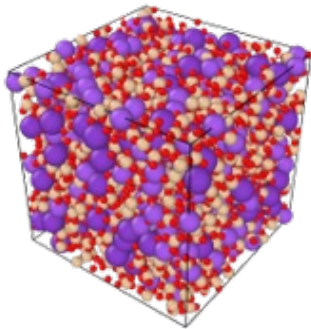


Time to result: days to weeks

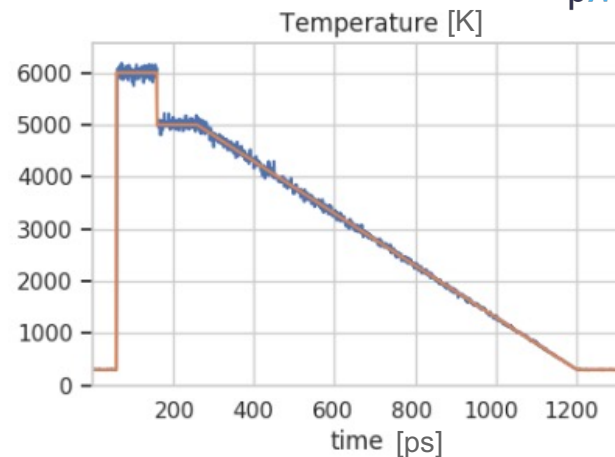
1. Simulation

1.2 Atomistic simulations

- Automated workflows for melt-quench procedure & property calculations
 - Using pyiron workflow manager
 - Targeting time to result: ~12h
- Classical & machine-learning force fields



Melt-quench workflow



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Chat Mockup

Glass Developer
Let's start development with the following three compositions: [...].

► Otto creates order for robotic melt.

Otto
Here are the melt orders with suggested raw materials.
[Download/View] Submit?

Glass Developer
That won't get done today anyway. Let's run the standard simulations overnight.

► Otto starts thermochemical melt simulations with GTT/FaCCT Sage.

► Otto starts atomistic simulations of glass composition and properties using universal ML potential. Runtime: 12 hours.

Otto
The simulated CTE for composition 3 deviates significantly from the target.

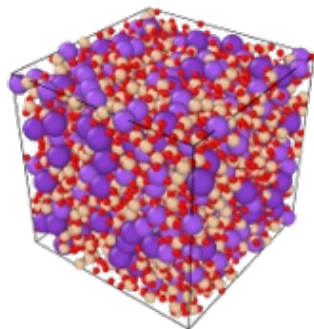
Glass Developer
Please submit the melt order for the other two compositions.

► Otto sends order to robotic melting facility.

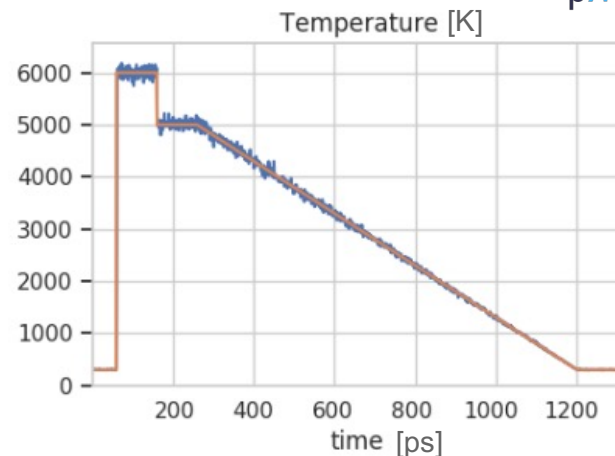
1. Simulation

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Melt-quench workflow



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Current work status

1. Workflow generation for:
 - Meltquench ✓
 - Viscosity ✓
 - Coefficient of thermal expansion ⌚
 - Elastic moduli ⌚
2. Structure analysis:
 - Radial distribution function ✓
 - Coordination numbers ✓
 - Bond angle distribution ✓
 - Q^n and Network connectivity (NMR-consistent structural metrics) ✓
 - Rings ✓
3. Classical potentials ✓
4. Development of ML potential ⌚

Plan to open-source classical potential workflows by April 2026 (& register them in PMD workflow store)

Demo – Atomistic simulation

- Using pyiron workflow manager
- Classical force field (PMMCS)

Chatbot

Property	Original Prediction	+5% Al ₂ O ₃ Prediction	Change
Refractive index (n _d)	1.547	1.543	-0.004
Abbe number	53.32	55.27	+1.95
CTE (ppm/K)	4.19	4.20	≈0

Interpretation:

- Increasing Al₂O₃ slightly **lowers refractive index** but **improves Abbe number**.
- CTE remains essentially unchanged.
- The model also predicts a small increase in Young's modulus and thermal shock resistance.

Do you want me to explore whether **further Al₂O₃ increases** could push the Abbe number above your target of 60 while keeping CTE low?

Message

I am interested in the atomic structure of this glass. Can you calculate it for me?

Clear Chat

Melt-Quench Simulation Results

Task ID: 50c135d3-8ffb-4822-ab54-f29bf0ed6aeb

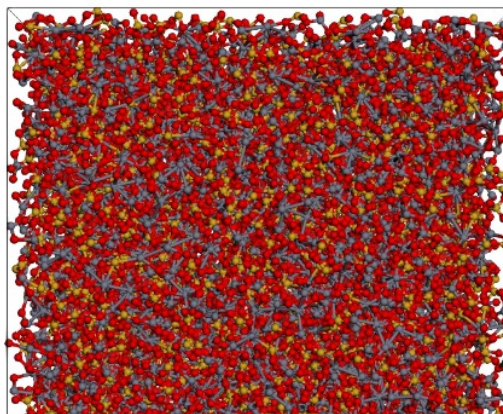
Composition: 0.25CaO-0.25Al₂O₃-0.5SiO₂

Atomic Structure

Style:

Ball & Stick ▾

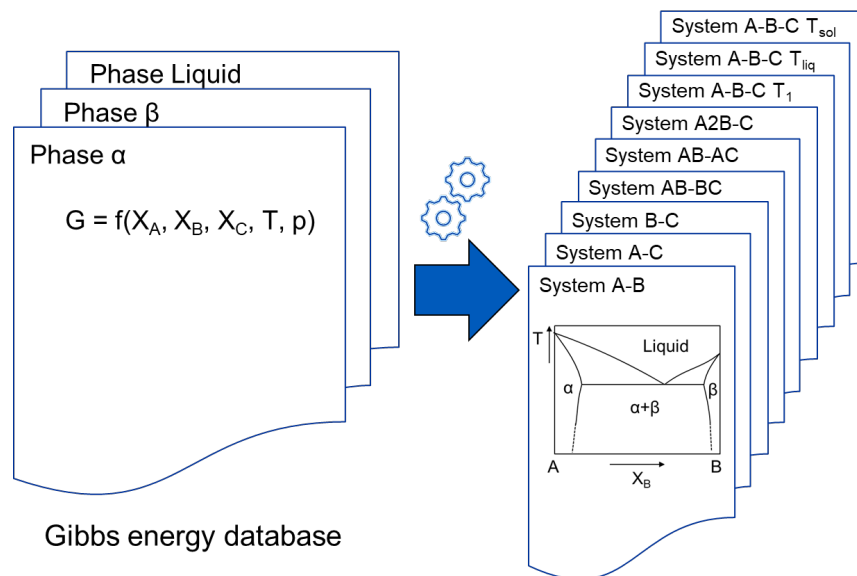
Reset View





1. Simulation

1.3 Thermochemical simulations (Calphad)



Gibbs energy database

Calphad = Calculation of Phase Diagrams

- Based on GTT's GTOx database & ChemApp software
- Current development focus:
 - Expansion of thermochemical database
 - Cloud-based software solution

Chat Mockup

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Here are the melt orders with suggested raw materials.
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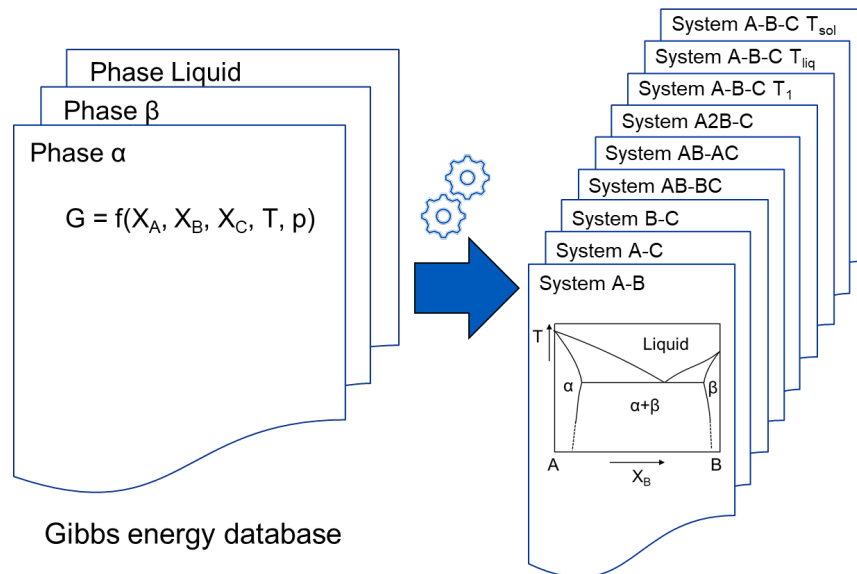
Otto
The simulated CTE for composition 3 deviates significantly from the target.

Glass Developer
Please submit the melt order for the other two compositions.

►Otto sends order to robotic melting facility.

1. Simulation

1.3 Thermochemical simulations (Calphad): overview and current work



Current work status

- Beta version of GTOx with B2O3 circulated
- Experiments on enthalpy of mixing ongoing at Schott
- Internal demo of cloud-based CalPhaD optimizer
- Prototype integration with GlasAgent

Calphad = Calculation of Phase Diagrams

- Based on GTT's GTOx database & ChemApp software
- Current development focus:
 - Expansion of thermochemical database
 - Cloud-based software solution

Demo – ChemSage liquidus line

- Using GTT ChemApp
- Feature: predict liquidus temperature along a one-dimensional composition range

Chatbot


- CaO solid
- CaCO₃
- CaSiO₃ polymorphs: wollastonite, pseudowollastonite
- Ca₂SiO₄ polymorphs: olivine γ, α', α, larnite (β)
- Ca₃SiO₅ (hatrurite)
- Ca₃Si₂O₇ (rankinite)

We can now:


- Run **equilibrium calculations** for any mixture of these components.
- Calculate **liquidus temperatures** along a composition axis.
- Explore **phase stability** over temperature/pressure ranges.

Do you want me to demonstrate an **equilibrium calculation** for a specific oxide mixture?

Message

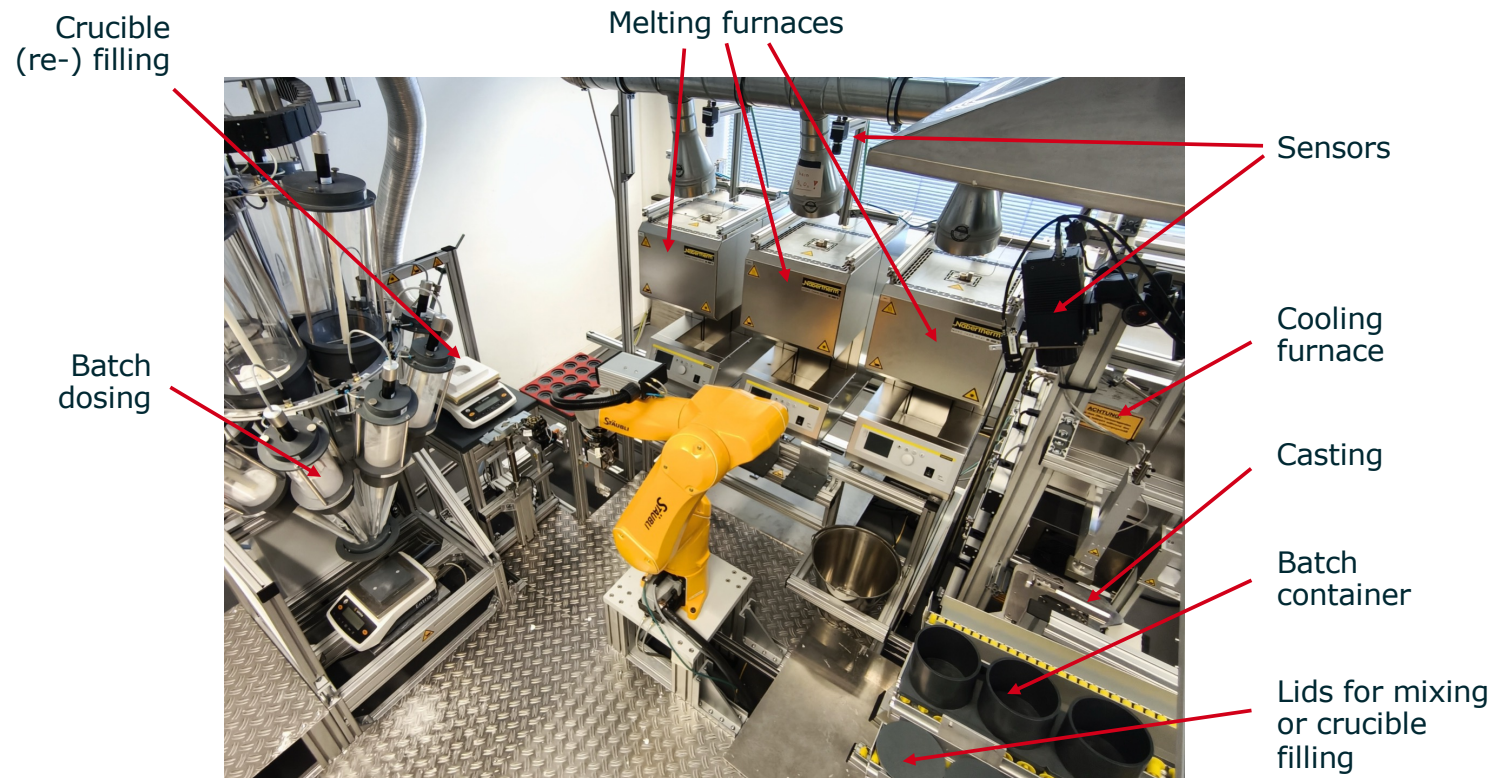


Let's start with a liquidus line. Show me how the liquidus temperature changes, going from silica to a typical soda-lime glass.



Clear Chat

2. Robotic Melting System: overview



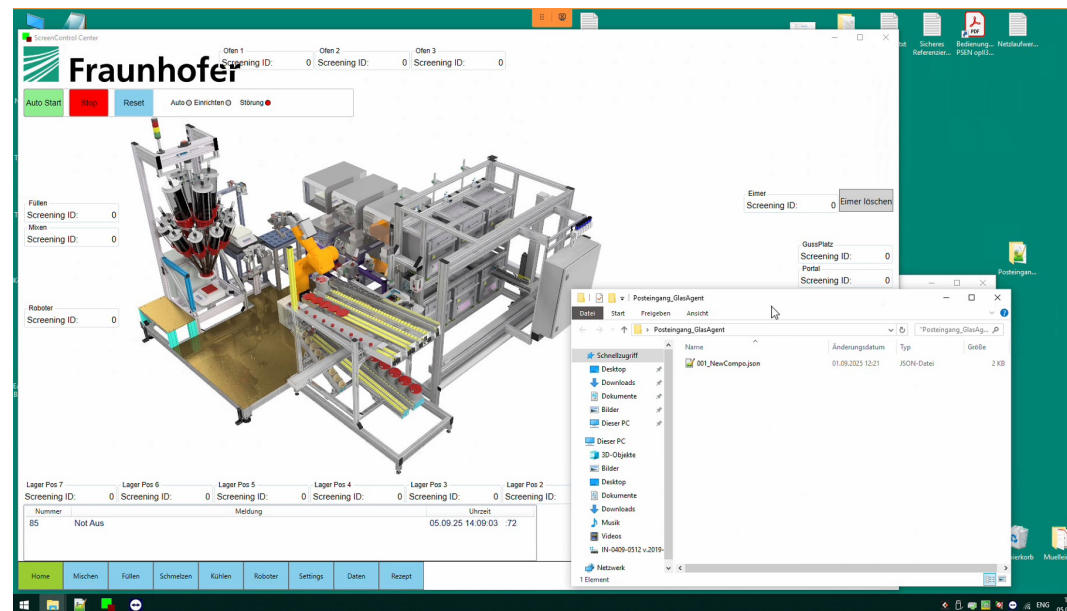
Goal: Step by step optimization

1. Automated definition of process parameters in the control software
2. Inline homogenization and measurement of viscosity & density

2. Robotic Melting System: current work

Implementation of automated definition of process parameters in the control software

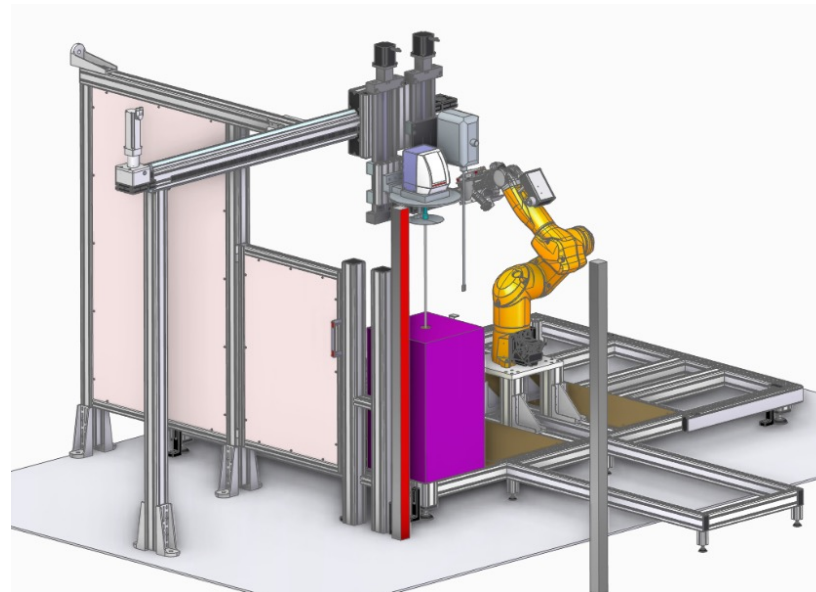
First milestone:
GlasAgent may electronically communicate melting orders to robotic melting system



2. Robotic Melting System: current work (continued)

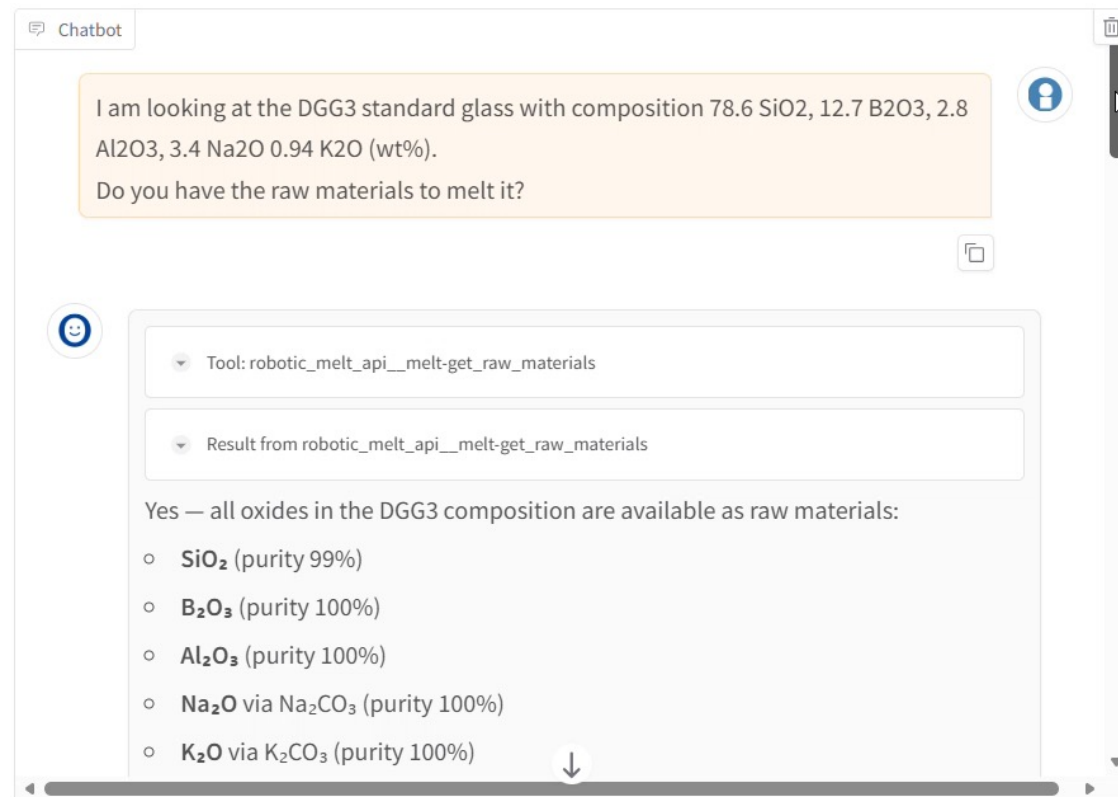
Inline Viscosimetry

- Construction of an **induction furnace**
 - with **stirring unit** for homogenizing the melt and
 - a **rheometer measuring head** for adjusting the viscosity before casting
- Improvement of reproducibility and quality of glass blocks



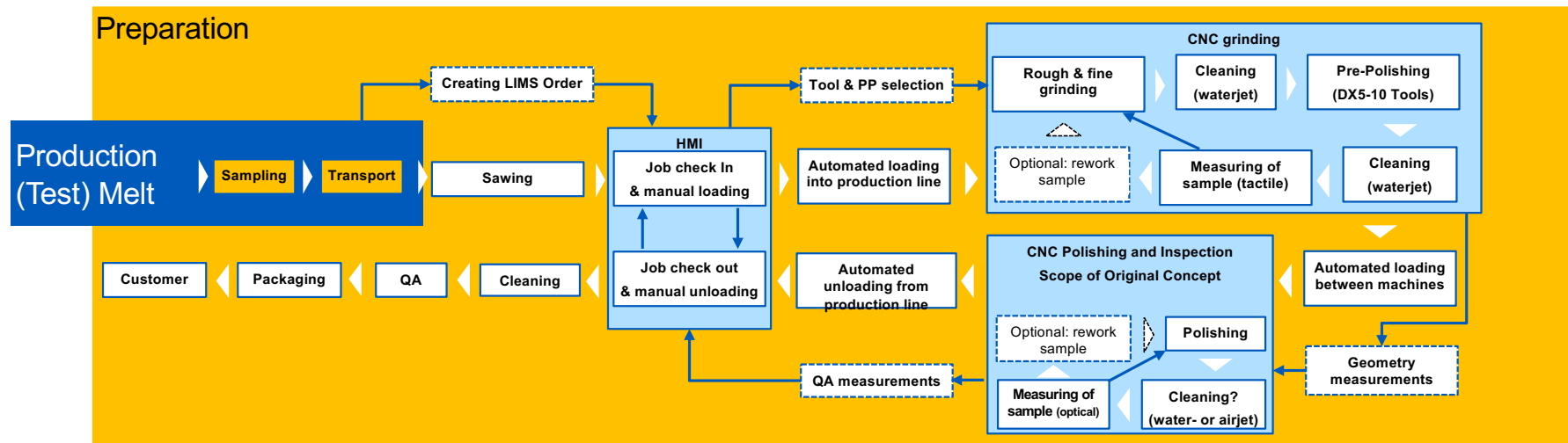
Demo – Submit melt request

- Using robotic melt API

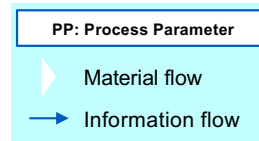


3. Automated Lab: bottleneck #1 sample polishing

3.1. Outline of a fully automated system



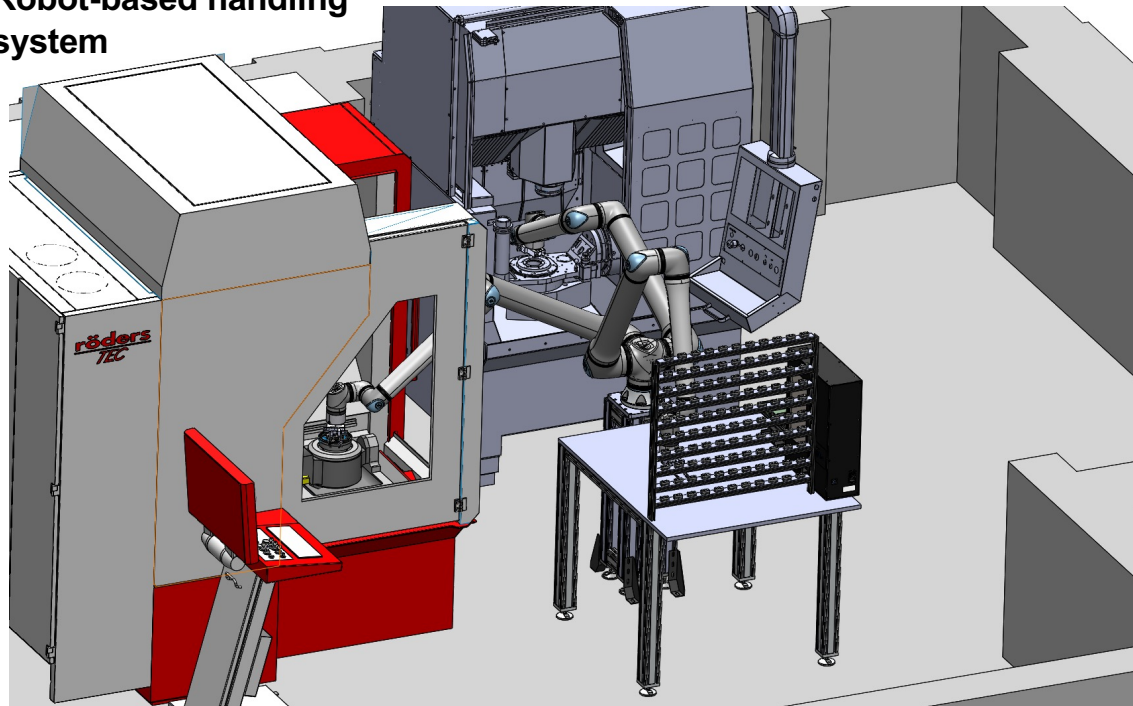
- Goals:**
1. Automated sample preparation for glass analysis: optical properties, chemical resistivity, mechanical strength, thermal properties; process time reduced to hours
 2. Required(1): robot-based handling system
 3. Required(2): camera-based automated quality control system for polishing processes



3. Automated Lab: bottleneck #1

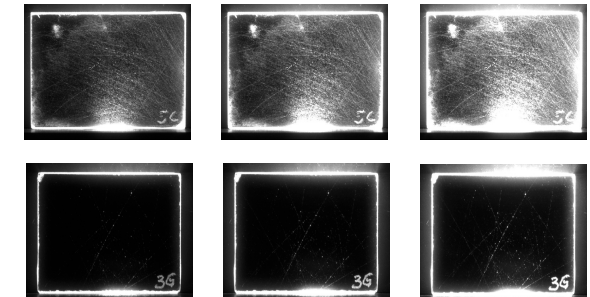
3.2 Some pictures

Robot-based handling system



Camera-based automated quality control system for polishing processes:

At which stage is the scattering at the surface so small that polishing is finished?



3. Automated Lab: bottleneck #2 wet chemistry

3.1 Idea: LIBS for quantitative glass analysis

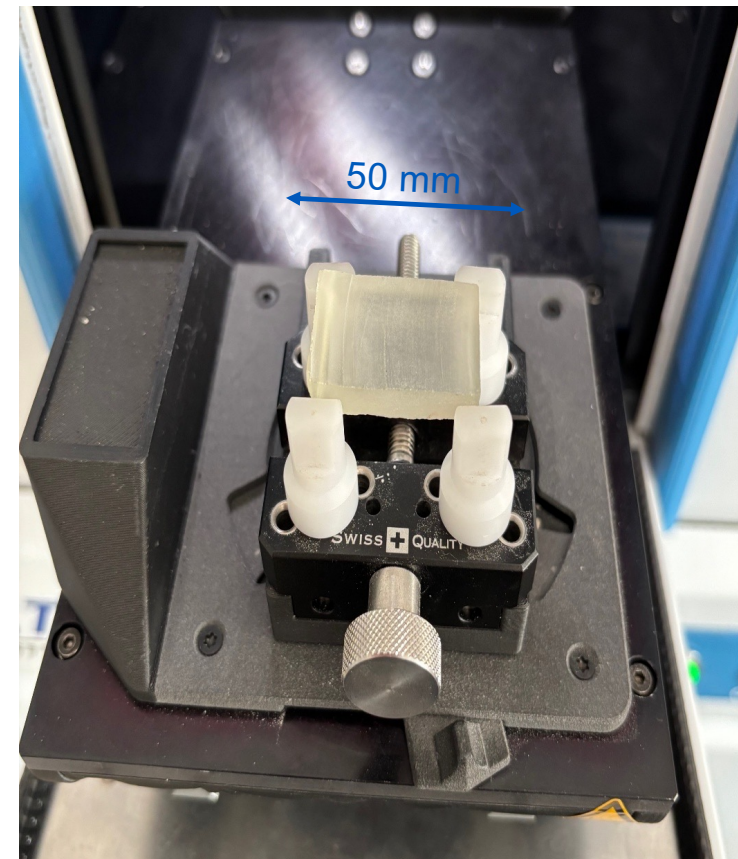
LIBS = Laser-Induced Breakdown Spectroscopy

Working Principle

1. Laser-Induced ablation, creating μm - to mm-size plasma
2. Optical emission spectroscopy of the plasma
3. Concentration of elements derived from intensity of characteristic spectral lines.

Goal

1. Feasibility of quantitative glass analysis
2. Replacement of wet chemistry



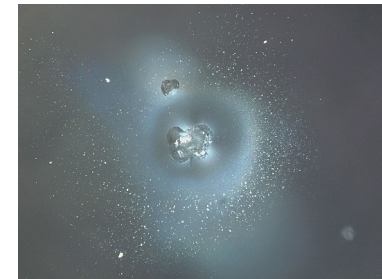
3. Automated Lab: bottleneck #2

3.2 Status of: LIBS for quantitative glass analysis

- LIBSpector arrived at BAM and under implementation
 - Integration in the robotic melting system necessary
- Oven for LIBS on melted glass is set-up in the LTB laboratory
 - New design of OEM-LIBS necessary
- First CAS glass calibration measurements with LIBSpector at BAM:
 - Repeat validation at the new location
 - Test for new CAS glass melts (CAS: Ca-Al-Si)
- Calibration on Borosilicate glasses was tested and laser parameters have to be changed to ensure similar impact on different glasses



undesired impact



desired impact

4. Production



MaterialDigital 3, Project GlasAgent

5. Product use at customer



6. Recycling

6.1. Separation of components from complex devices

- Innovative company specializing in various recycling technologies
- Broad product portfolio: Impact Crushers, Hammer Mills, Shredders, Screening and Sorting Systems

Areas of Application:



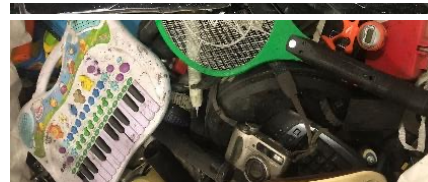
SOLAR



LAMINATED GLASS



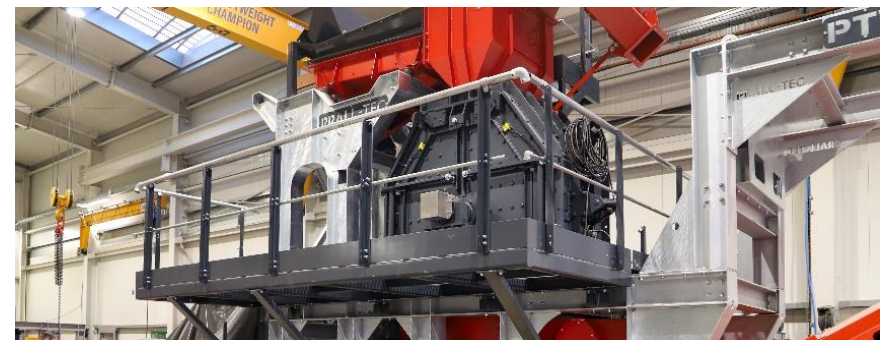
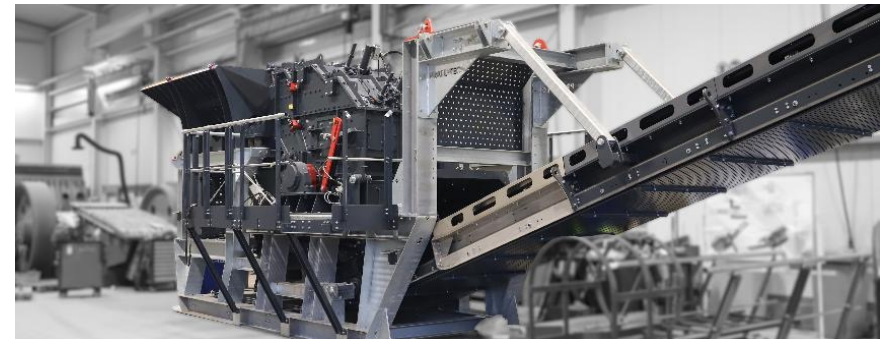
FLOAT GLASS



E-SCRAP

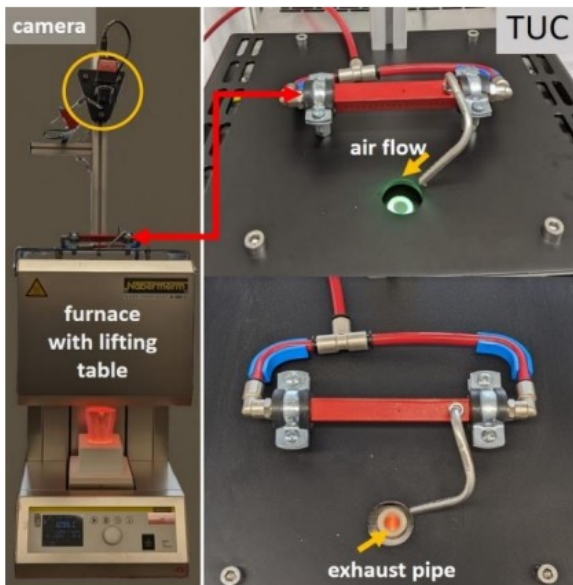
PRALL-TEC

Plant Engineering:

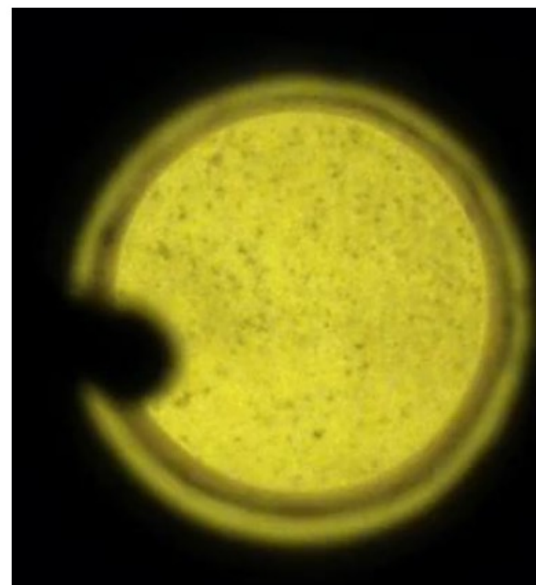


6. Recycling

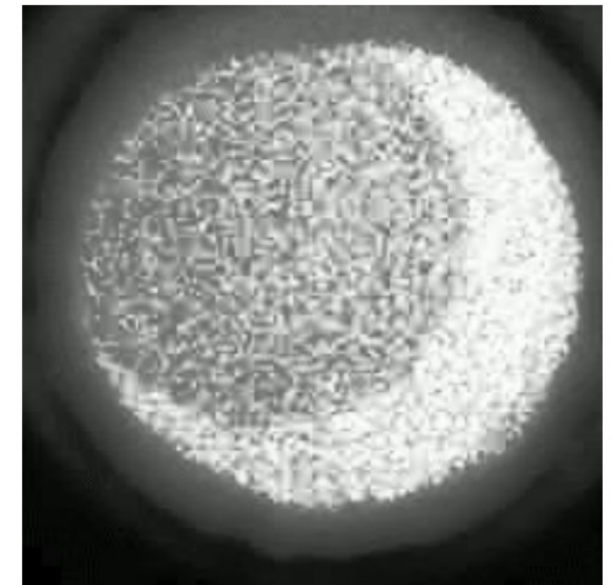
6.2. Test of melting behaviour



Electrical furnace with a **camera**
Monitoring through a narrow
 Al_2O_3 tube



ML- Image analysis
Melt stages (ResNet34)
Granules → Foaming → Fining

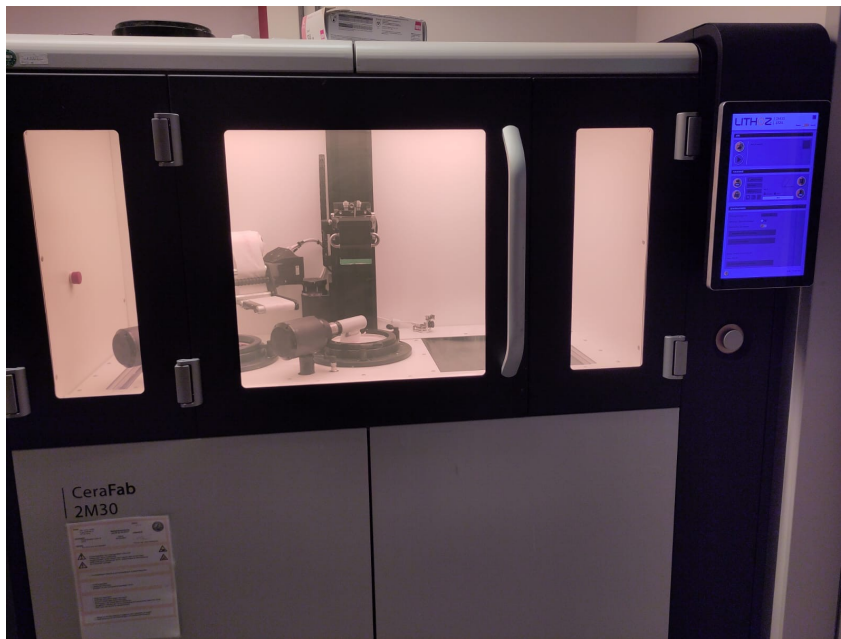


ML- Image analysis
Castability check (Mechanical impact →
Image change rate reflects viscosity)*

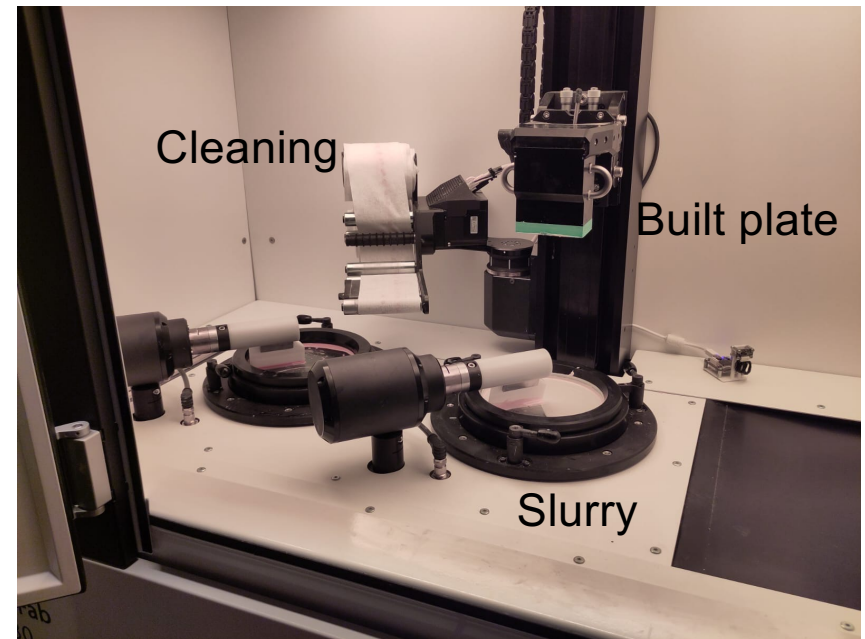
6. Recycling

6.3. High-Throughput Glass Characterization

3D printer



Multi-component printing



6. Recycling

6.3. High-Throughput Glass Characterization

First step is a 3D-print of a suitable slurry consisting of glass precursors and organics

Second, organics get burned off and glasses with different compositions remain

Next step is upscaling the process to the desired sample amount

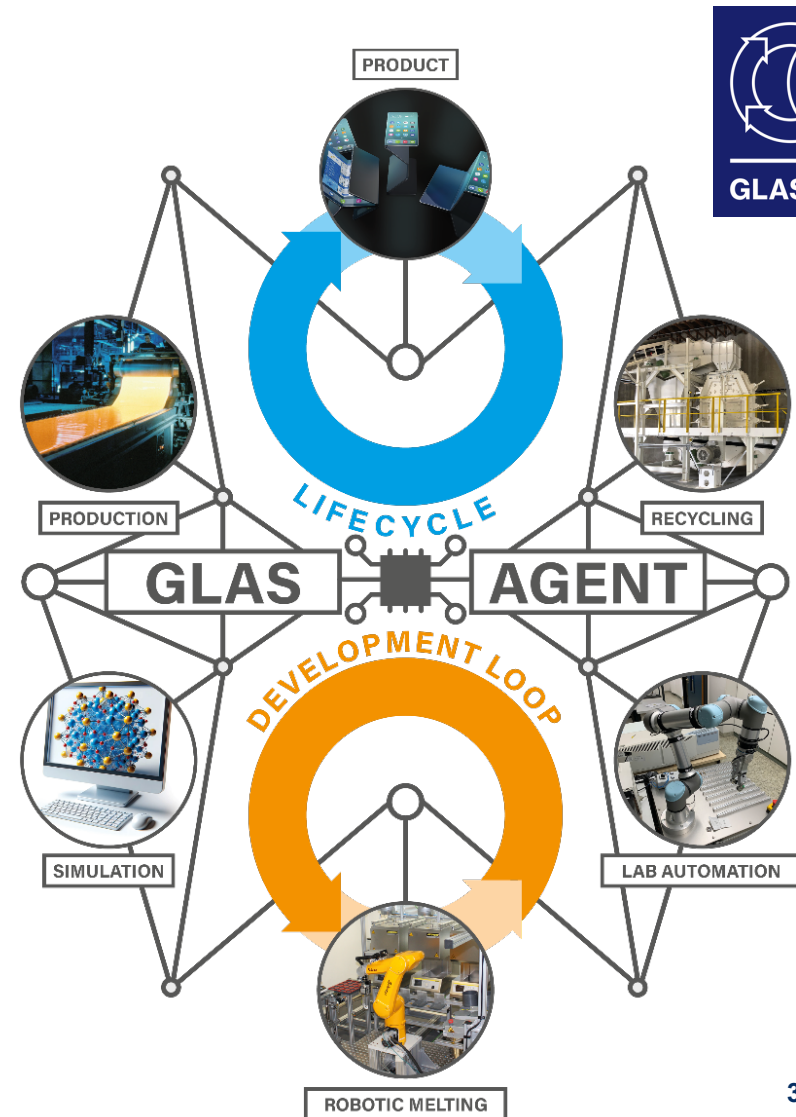
Current working is on ways of characterizing the quality and reliability of the print



GlasAgent

- **Goal 1:** accelerate specialty glass development through
 - Easy-to-use digital tools via chatbot interface
 - Automatic simulation workflows
 - Robotic melting system
 - Sample preparation for any analysis by automated polishing
 - LIBS for fast composition measurement
 - Demonstrator: development of special glass for optoelectronics
- **Goal 2:** enable recycling of special glasses & integrate it into the development process
- **Partners:** 10 partners from industry, university & research institutes with leading expertise
- **Duration:** 01/2025 - 12/2029

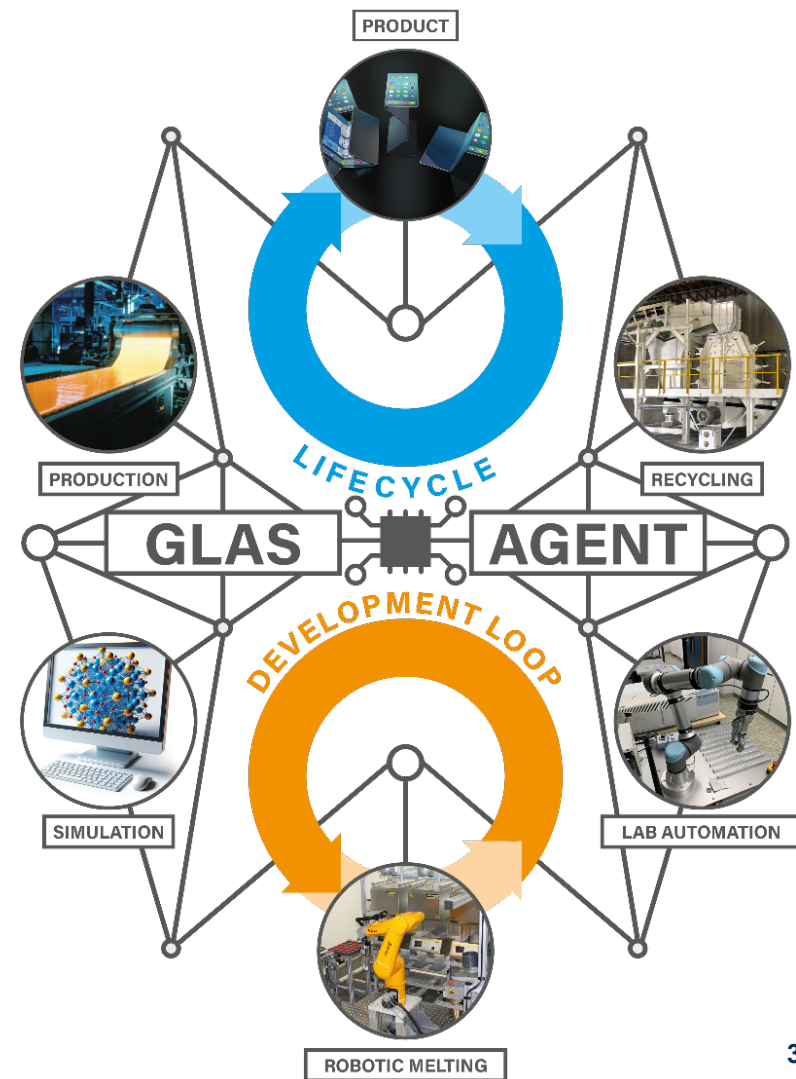
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GlasAgent says “Thank you” to

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Discussion

