Glass Synthesis in the Digital Age

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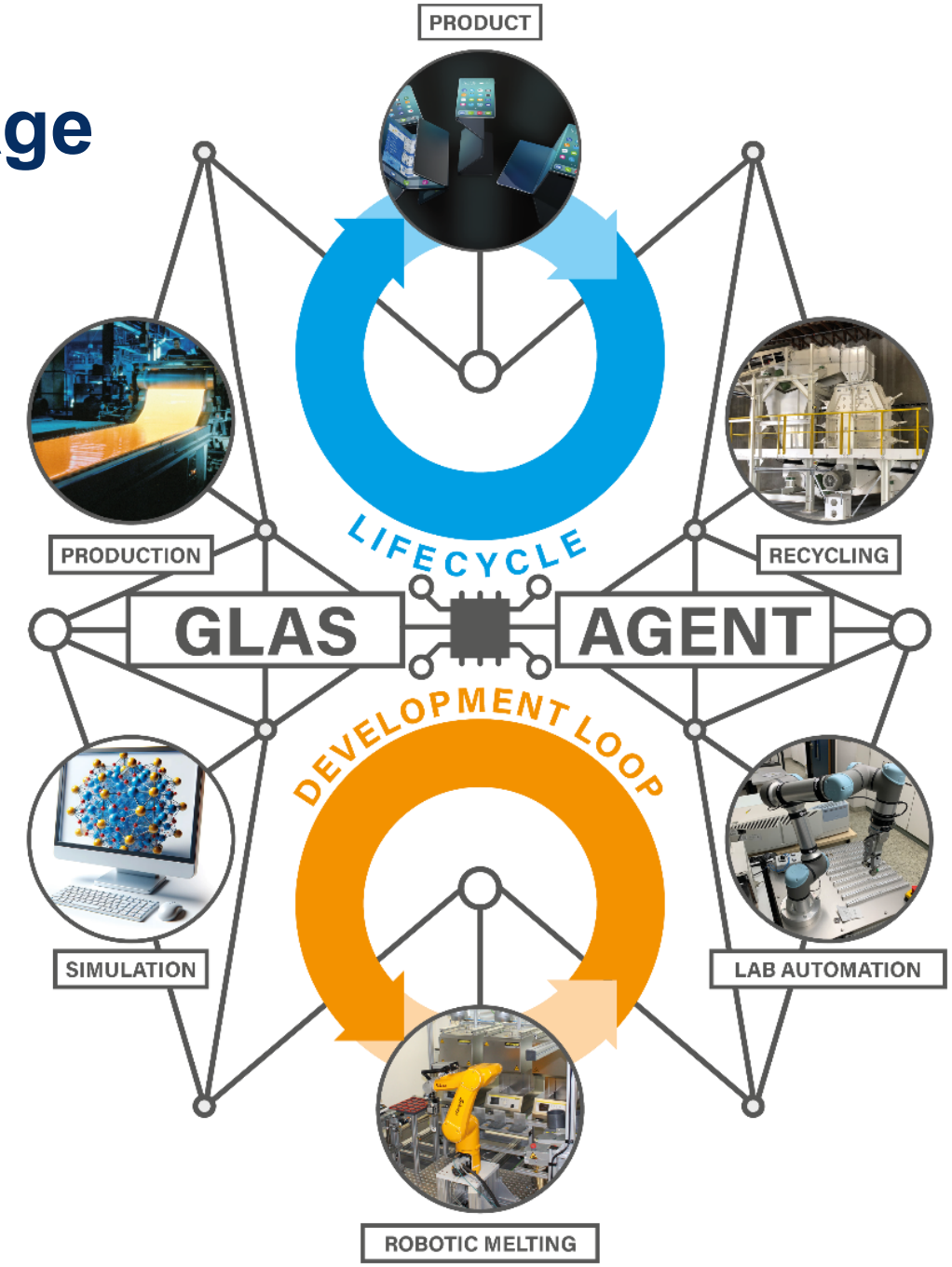


Vision for Specialty Glass Development and Life Cycle

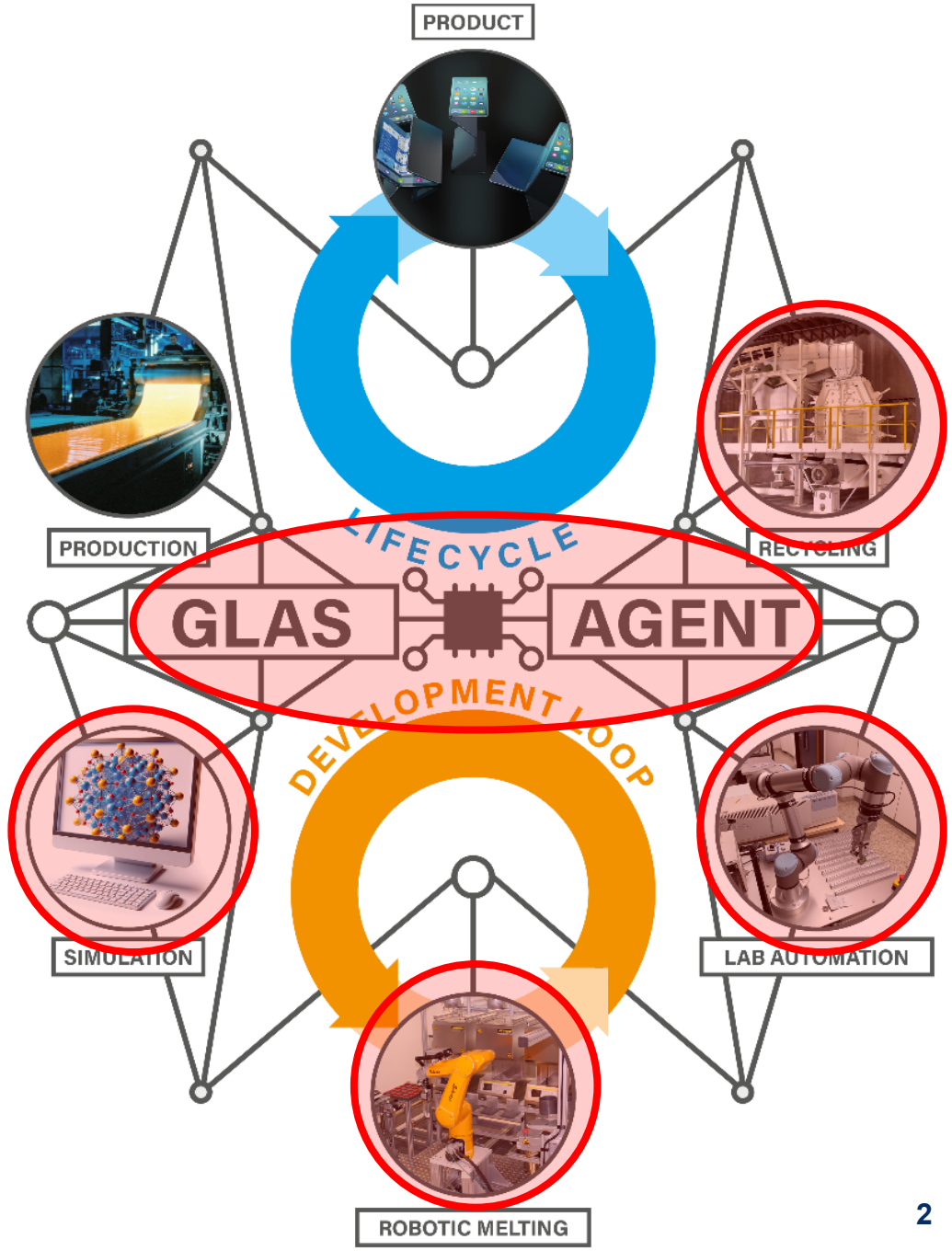
Glass Development Loop

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

GlasAgent: Software agent integrating these loops

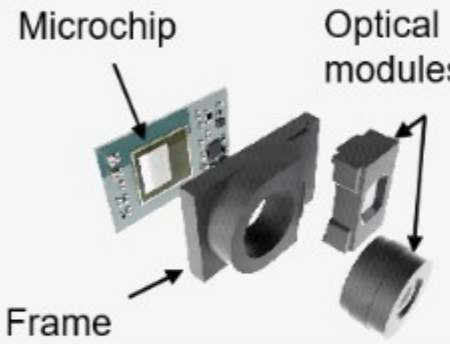


Application

New specialty glass for cost-effective optoelectronic components

State of the art

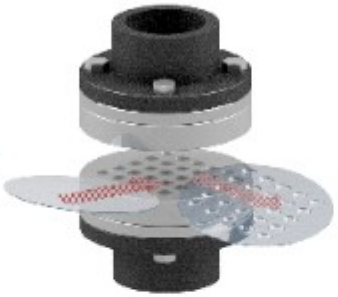
Multi-step assembly process of Individual components



Optical manufacturing and micro assembly are **cost drivers** for MEMS packages

Approach

Optic manufacturing



Precision glass molding at 4 to 12 inch wafer-level

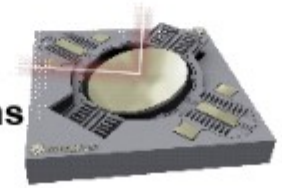
Packaging

Wafer-level assembly of glass encapsulation and MEMS wafers

MEMS design

Optimized MEMS design

Miniaturized MEMS Mirror Scanners for AR/VR Applications

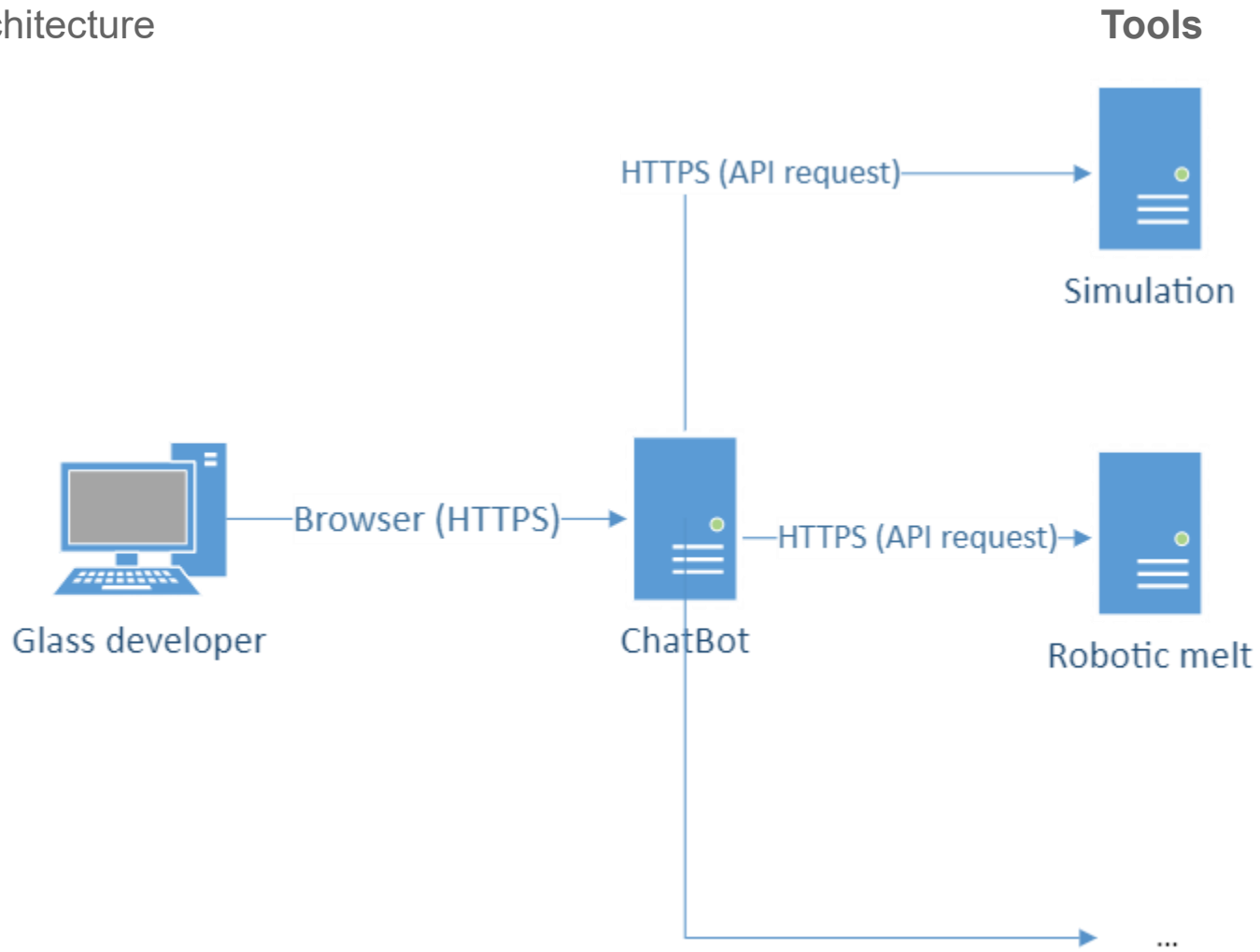


Head-up-Display

Head-Mounted Display

GlasAgent

Architecture



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

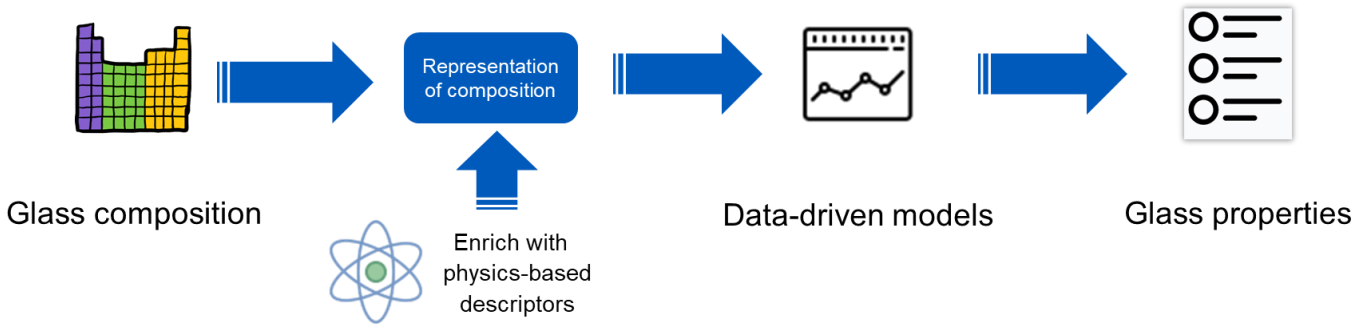
Unfortunately, I couldn't find any known glass with those properties. Should we try inverse design?

Glass Developer

Yes, let's give that a try.

1. Simulation

1.1 Data-driven models



- Given **composition** (75% SiO_2,15% Na_2O, 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.

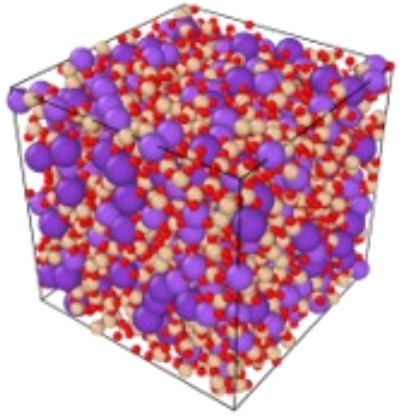
Glass Developer
That's not a bad start. What's the prediction if I increase component X by 1% and omit expensive components?

▶Otto uses the FancyML model for prediction

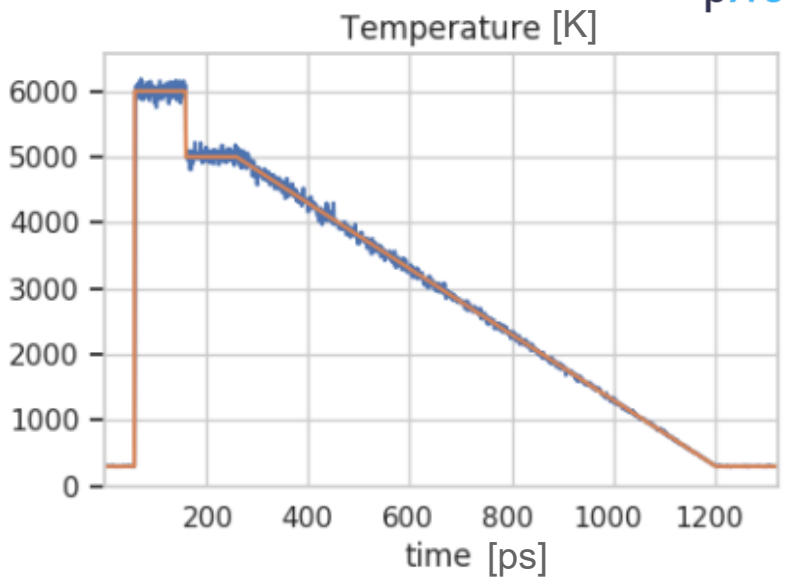
1. Simulation

1.2 Atomistic simulations

- Automated workflows for melt-quench procedure & property calculations
- Classical & machine-learning force fields
- Using pyiron workflow manager



Melt-quench workflow



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.*

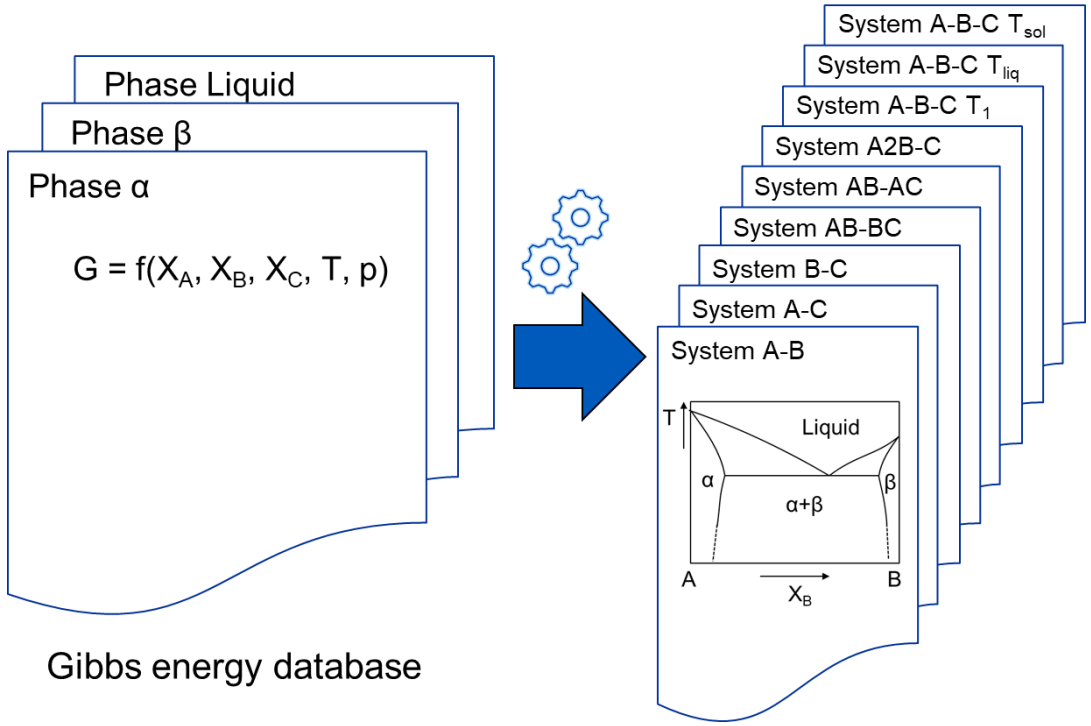
Otto
The simulated CTE for composition 3 deviates significantly from the target.

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

▶*Otto sends order to robotic melting facility.*

1. Simulation

1.3 Thermochemical simulations (Calphad)



Calphad = ***Cal*culation of *Pha*se *D*iagrams**

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

Chat Mockup

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

▶*Otto creates order for robotic melt.*

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Here are the melt orders with suggested raw materials.
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That won't get done today anyway. Let's run the standard simulations overnight.

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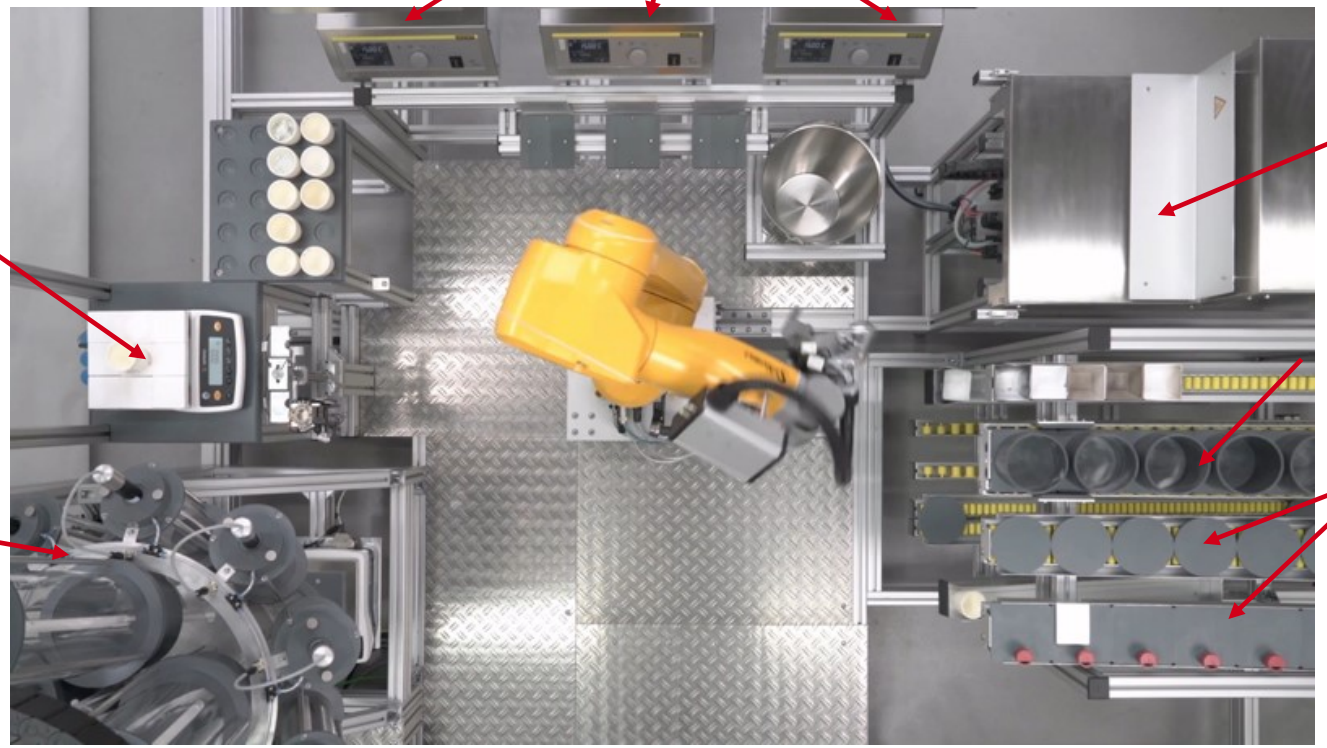
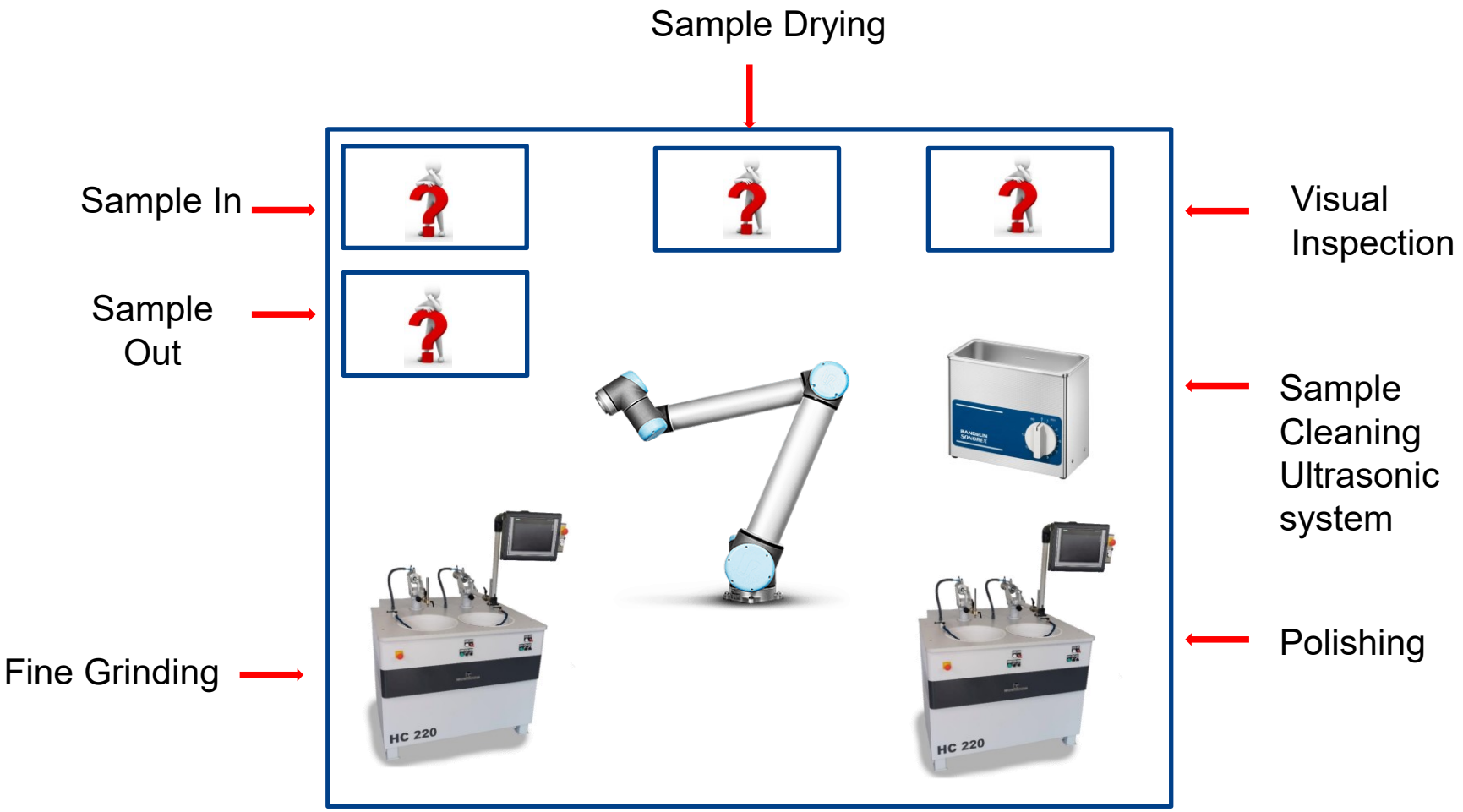
2. Robotic Melting System



Development Goals

1. **Automated definition of process parameters in the control software**
2. **In-line measurement of viscosity & density**

3. Automated Lab
3.1. Sample Polishing (bottleneck for various tests)



Development Goals

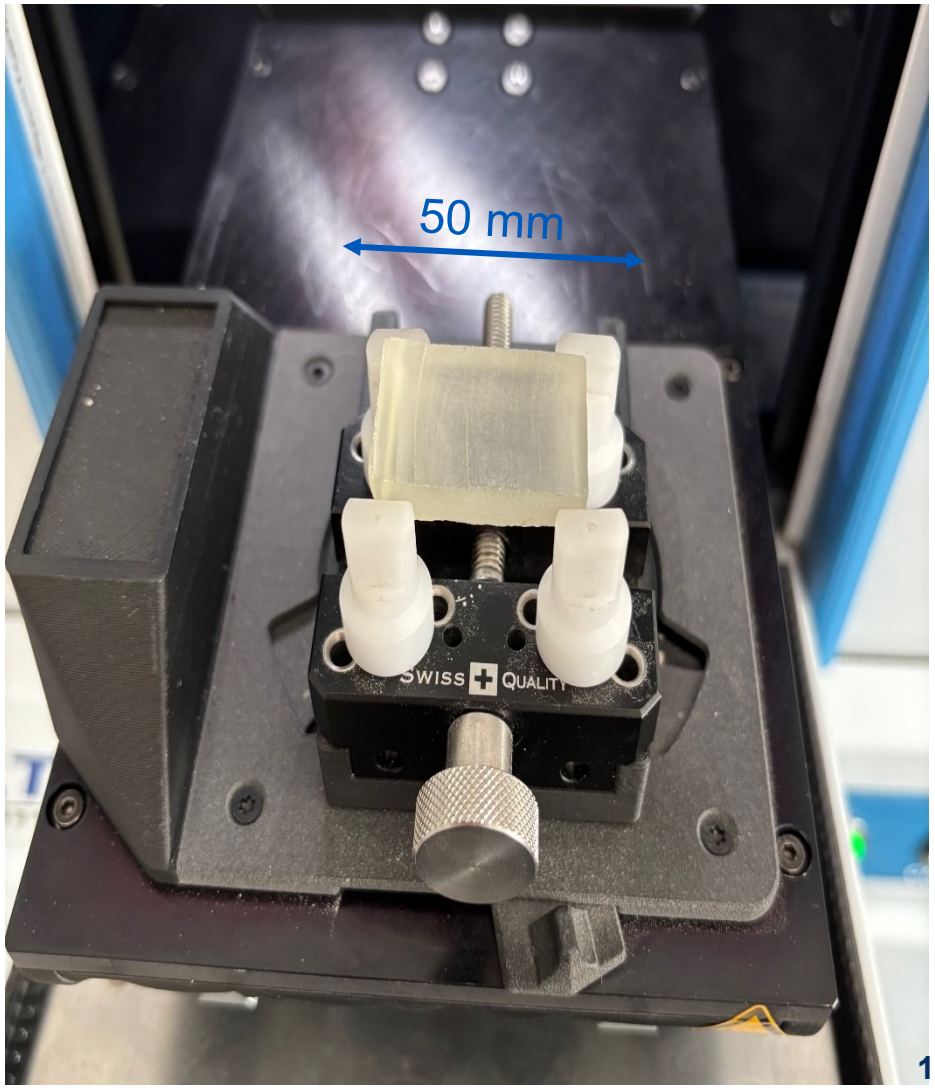
1. **Development of a robot-based system for automated sample preparation in glass analysis**
2. **Development of a camera-based automated quality control system for polishing processes**

3. Automated Lab
3.2.1 LIBS for quantitative glass analysis

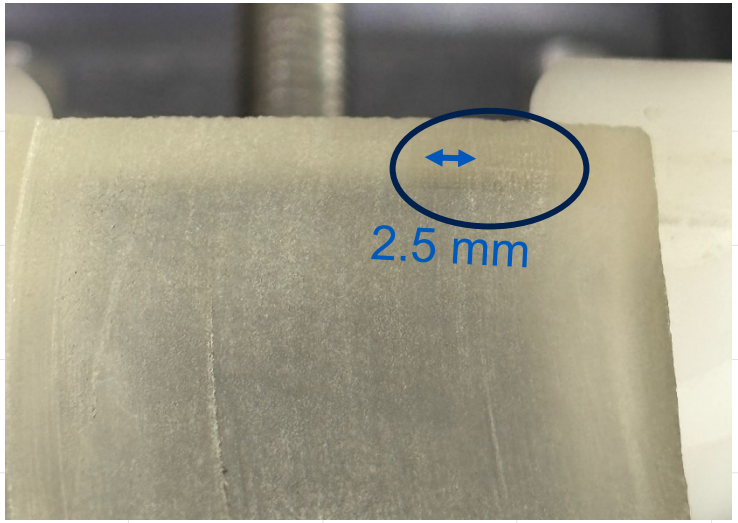
LIBS = Laser-Induced Breakdown Spectroscopy

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.



3. Automated Lab
3.2.2 LIBS for quantitative glass analysis



CALIBSO settings

Diode pumped ns-laser:
1064 nm, 4 mJ – 24,5 mJ

Spectrometer:
210 nm – 850 nm

Settings:
10 x 10 grid on 2.5mm x 2.5mm area
0 – 20 cleaning shots.
10 shots accumulated on camera

Glass sample with **three** main components:

Al_2O_3, SiO_2, CaO

CALIBSO LIBS experiment on rough, sawn side

4. Production

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:

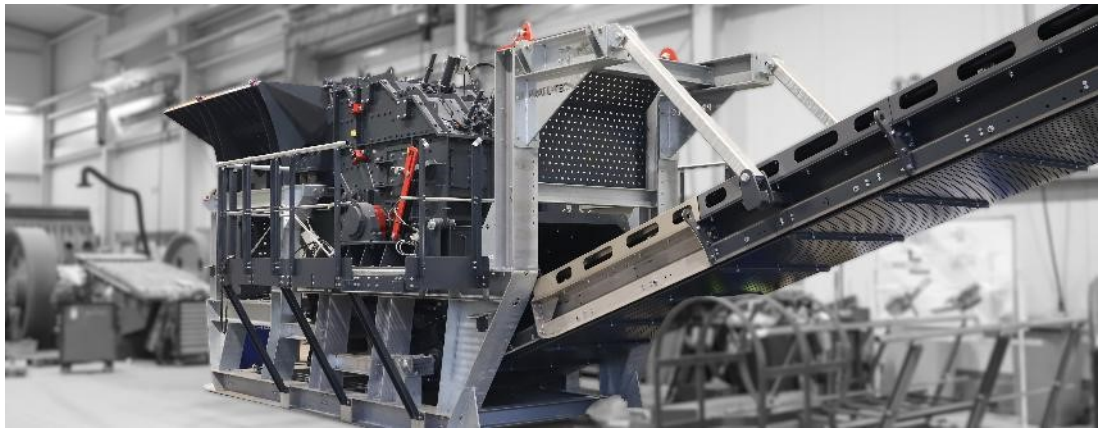
SOLAR

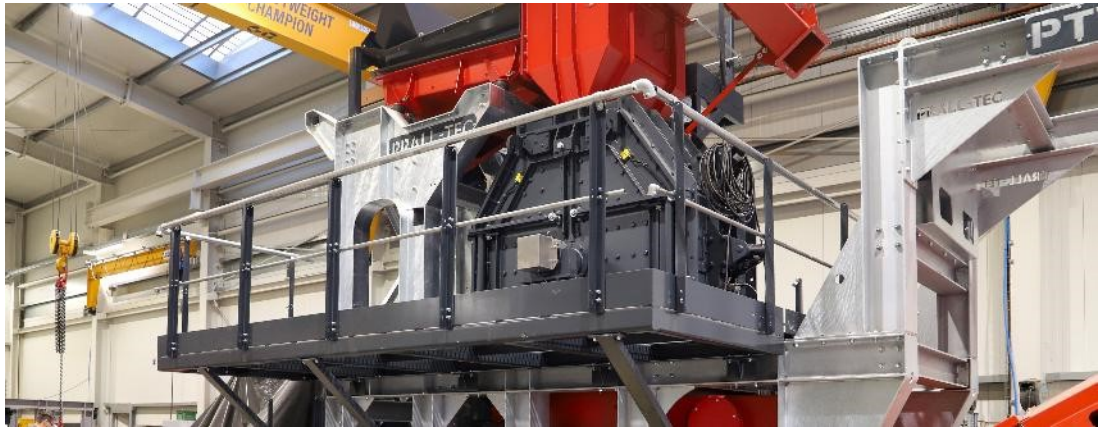
LAMINATED GLASS

FLOAT GLASS

E-SCRAP

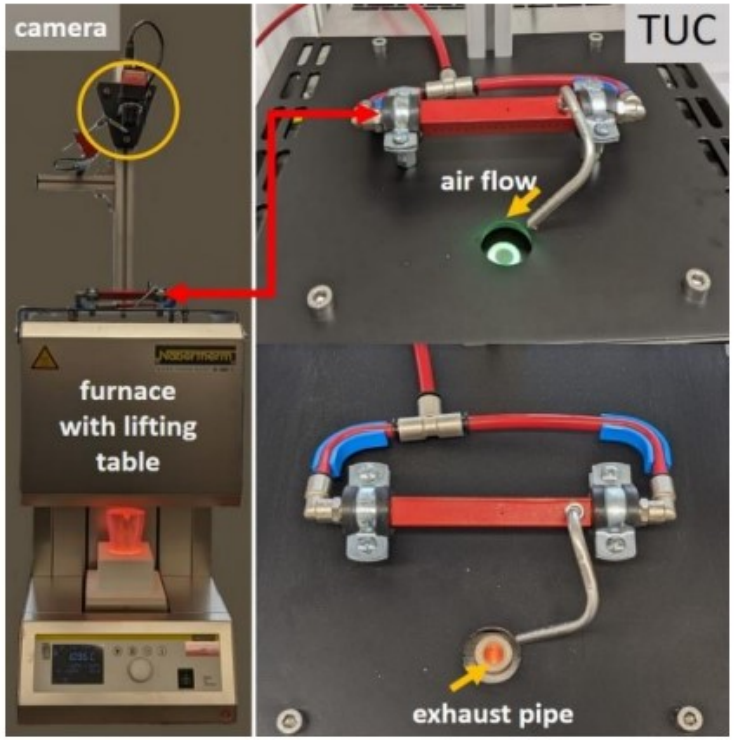
Plant Engineering:



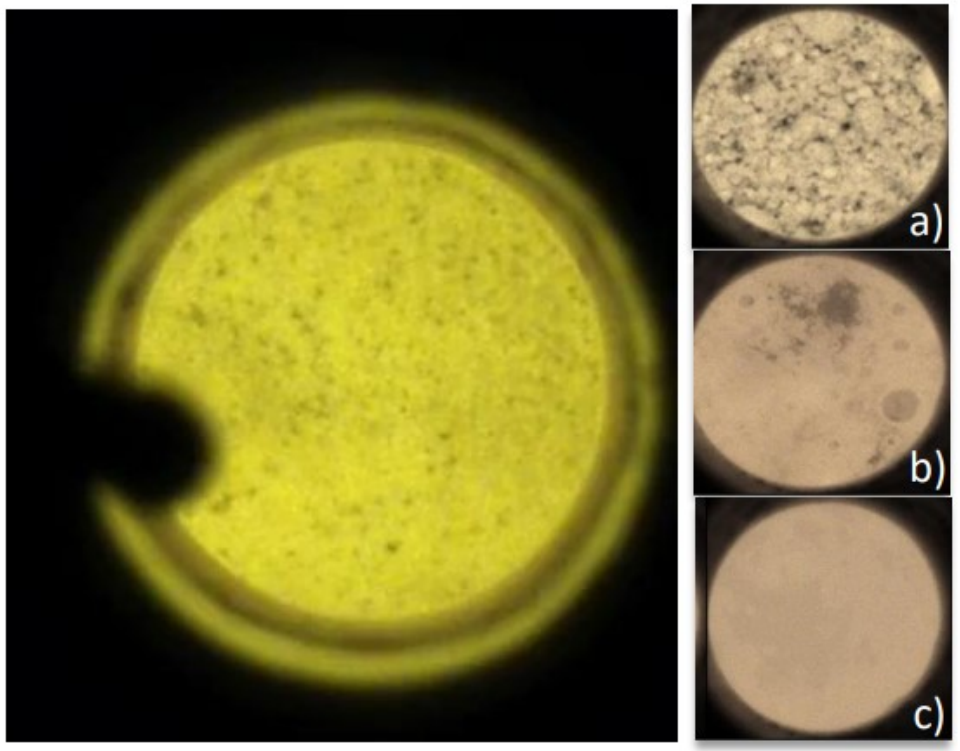


MaterialDigital 3, Project GlasAgent

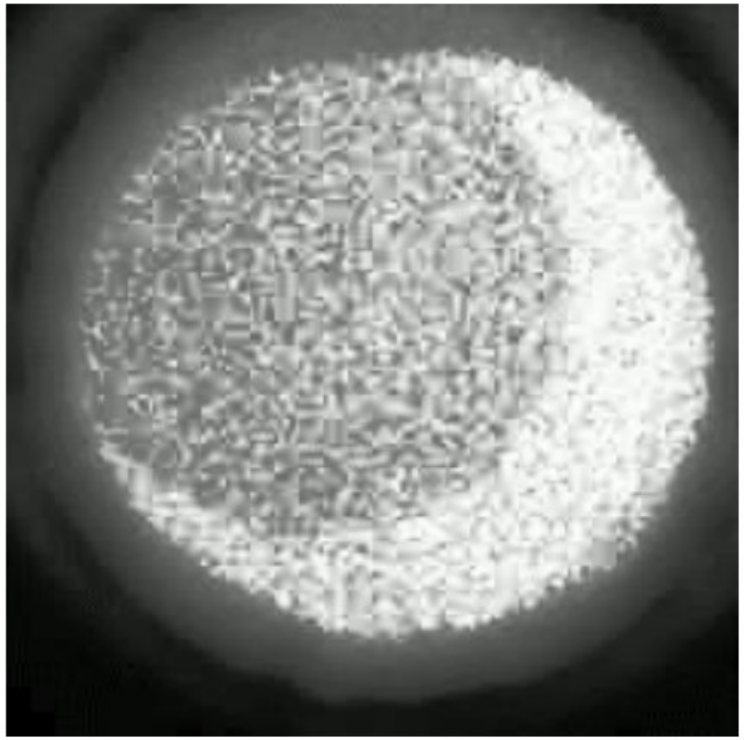
6. Recycling
6.2. Test of melting behaviour



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



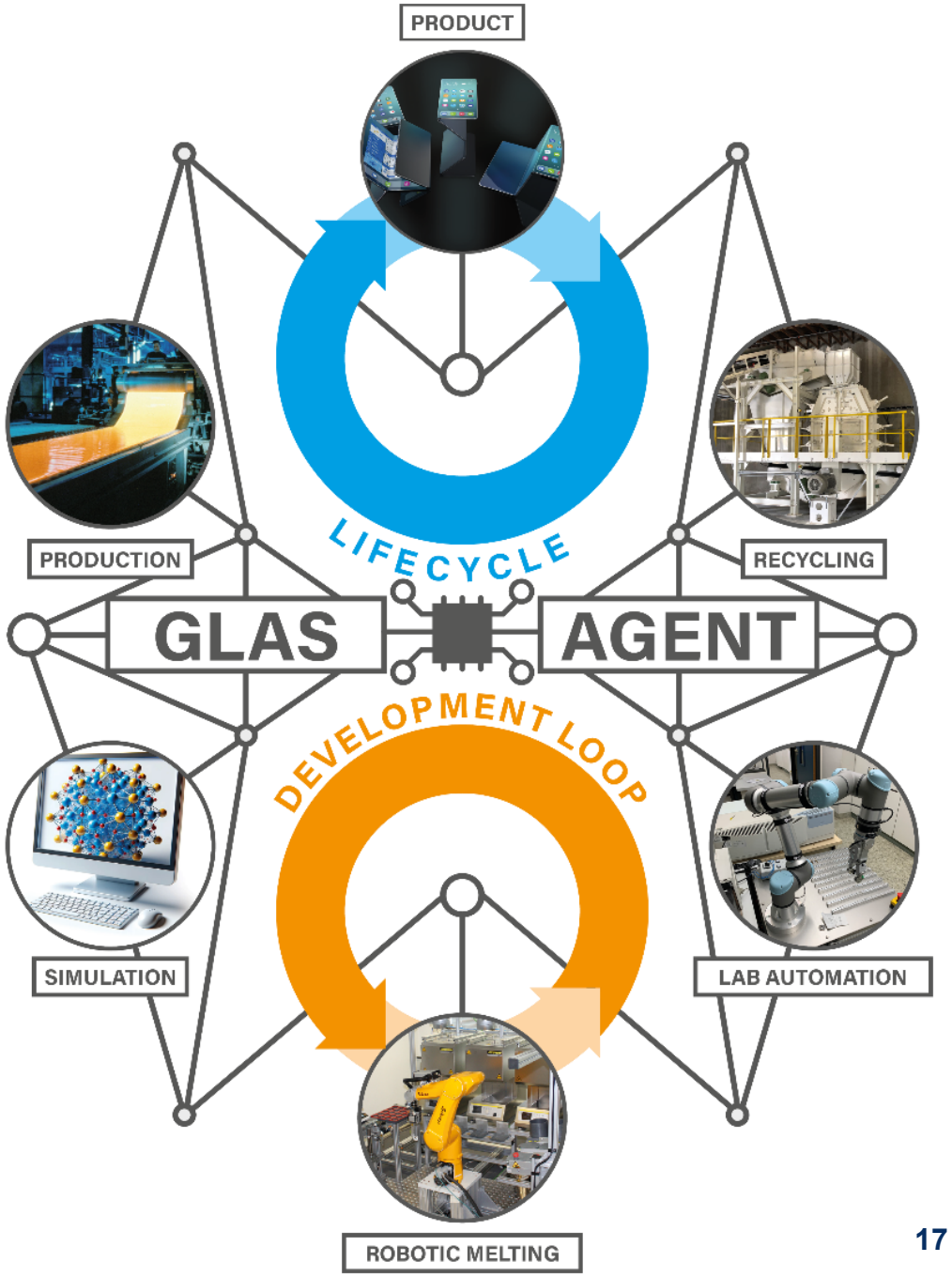
ML- Image analysis
Melt stages (ResNet34)
Granules → Foaming → Fining



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

GlasAgent

- **Goal 1:** speed up specialty glass development through
  - Easy-to-use digital tools via chatbot interface
  - Automatic simulation workflows
  - Robotic melt
  - 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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Discussion

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