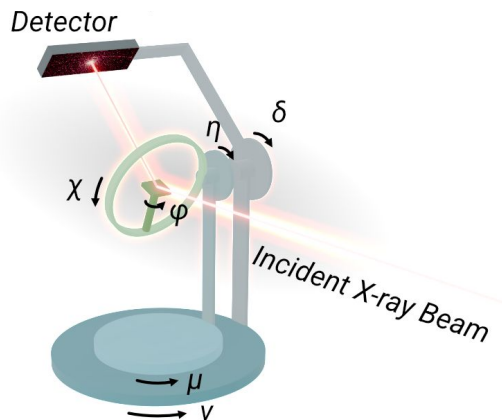


Toward Automated X-Ray Experiments

An Inspectable Language-Model Sub-Agent for Bragg Peak Centering

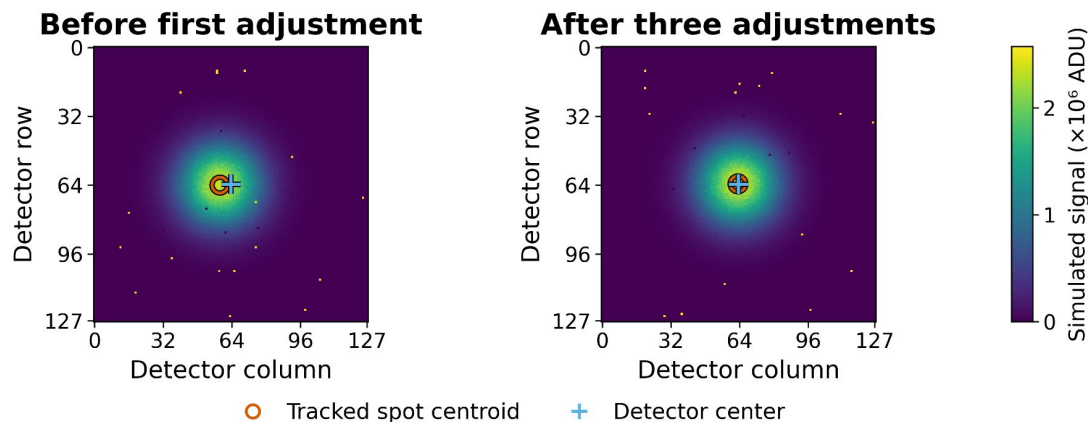
David Katz, Elias Stengel-Eskin, Zhantao Chen • The University of Texas at Austin

Bragg peaks are sharp X-ray diffraction signals that reveal the regular, repeating arrangement of atoms in a crystalline material.



6-Circle Diffractometer

Our task: center one selected spot by adjusting two simulated motor axes.



Reconstructed detector images from one recorded simulation episode.

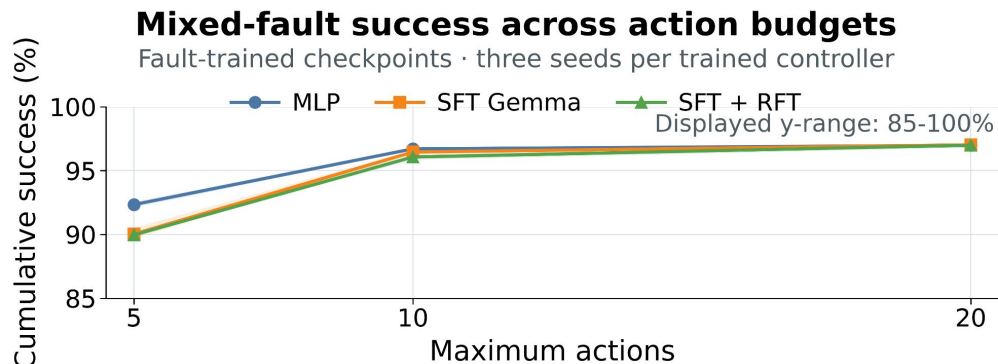
Can a small language model learn a laboratory control skill?

"Instrument: AI-assisted X-ray alignment"

Source: Reprinted from Chen et al., Nat. Mach. Intell. (2026),

DOI: 10.1038/s42256-026-01261-5

Fine-tuning enabled simulated centering



≈97% success within 20 actions

Mixed-fault development evaluation

Comparable to a compact neural-network baseline

Computer vision measures the spot position.

Gemma proposes the next motor adjustment.

Python checks movement limits before the simulator executes accepted moves.

The loop repeats with the next measurement.

