Team eJect
Hack the Microscope 2025

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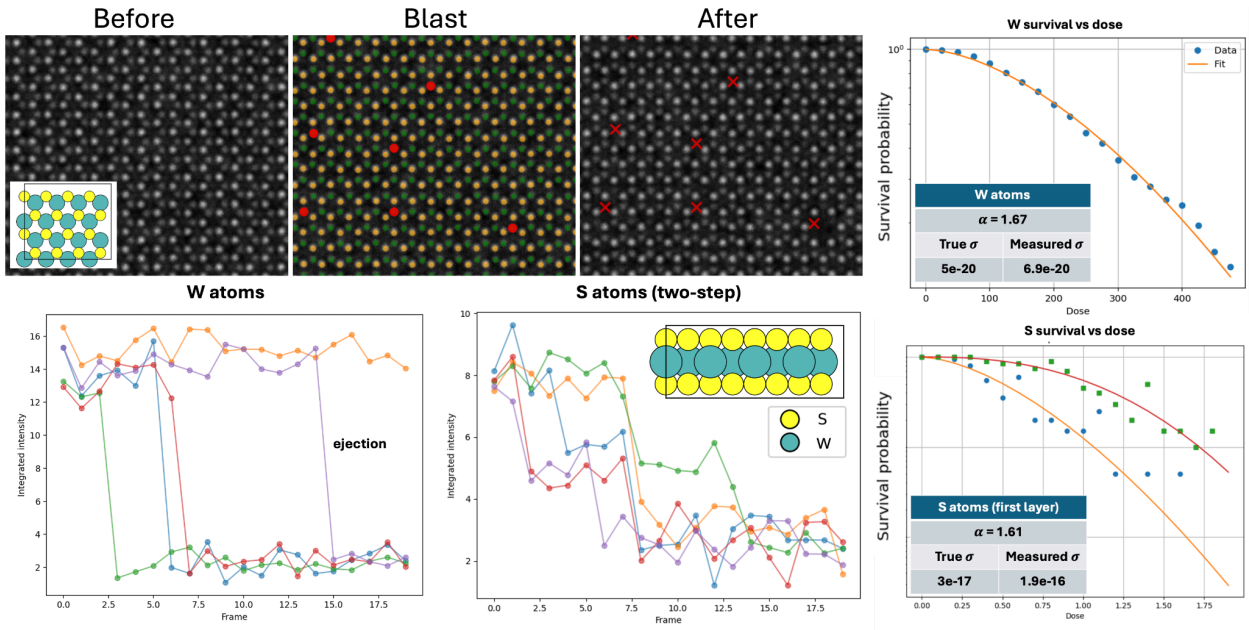
Aberration-corrected scanning transmission electron microscopy (STEM) has advanced beyond passive imaging to become an active tool for modifying matter at the atomic scale. A highly focused electron probe can displace atoms, drive bond rearrangements, and induce localized phase transformations through a combination of knock-on collisions, electronic excitations, and beam-stimulated chemistry. While these processes are often described collectively as “beam damage,” they can also be harnessed for controlled atom manipulation and nanoscale fabrication when delivered with sufficient spatial, temporal, and dose precision. However, the stochastic nature of beam–matter interactions and the difficulty of disentangling competing mechanisms have limited the development of predictive, reproducible atom-scale experiments.

We present a digital twin framework for quantitative atom manipulation in aberration-corrected STEM and validate it experimentally on a monolayer WS_2 sample using a ThermoFisher Spectra 300 at the University of Tennessee, Knoxville. The digital twin emulates realistic microscope operation through asynchronous client–server communication and incorporates a stochastic, physics-based beam–matter interaction model in which atomic modifications are driven by accumulated electron dose. This design enables direct transfer of experimental protocols from simulation to a physical microscope without modification.

Using the digital twin, we perform blind point and blast irradiation experiments, remaining agnostic to the physical constants used internally by the simulator, and identify atom ejection events by monitoring changes in atomic intensity. Atom loss is readily detected for high-Z species such as tungsten, while removal of sulfur atoms is more challenging due to stacked atomic columns and overlapping intensity contributions in WS_2. By tracking the number of remaining atoms as a function of accumulated dose, we extract survival curves that are well described by two physically meaningful contributions. The first term corresponds to ballistic (knock-on) damage and increases linearly with dose, while the second term captures non-ballistic mechanisms that, in the simulator, arise from dose-dependent structural instability that modifies the effective interaction cross section.

Survival (y-axis) | Ballistic Damage | Other Damage

$$S(D) = \exp[-(\sigma D + AD^{\alpha})]$$



Fitting this model yields estimates of the effective displacement cross section, σ, for each atomic species to within an order of magnitude. The non-ballistic term is characterized by an exponent α slightly greater than one, indicating a weakly superlinear—effectively exponential—increase in damage susceptibility with dose. We then applied the same digital-twin-derived protocol on the real microscope. Due to time constraints, only five experimental data points were collected, resulting in an uncertainty of approximately two orders of magnitude in σ. Despite this limitation, the fitted α decreases by ~0.2 relative to the simulator, suggesting a stronger contribution from damage mechanisms that accumulate linearly with dose, such as radiolysis, under experimental conditions. This comparison demonstrates both the realism of the digital twin and its ability to expose discrepancies that guide future model refinement and targeted data collection.

Having thoroughly characterized the ballistic damage contribution, we next focus on the non-ballistic damage term by drilling beam-induced holes and tracking survival statistics as a function of local coordination, which serves as a measure of structural instability. Future work will extend these experiments to larger batches and datasets to improve statistical confidence and more fully quantify nonlinear damage mechanisms in real material systems.