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Dynamics of He Bubbles during Thermal Annealing: A Data-driven Approach

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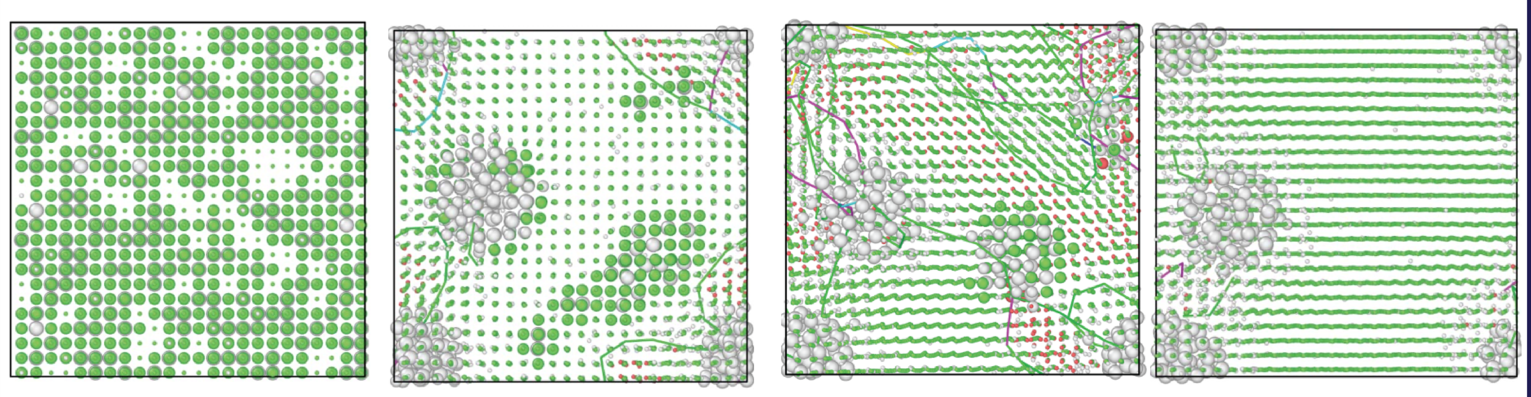
IntroductDataset and Pre-analysis

Introduction to the Dataset:

Pd metal with He implants at 400°C, followed by a thermal anneal at 500°C, 550°C, 600°C, and 650°C.

- Materials designed for nuclear reactor environments must perform under extreme conditions, including radiation damage, elevated temperature, and mechanical stress. He is generated through nuclear reactions and is insoluble in most materials. He bubbles that coalesce to cavities can degrade properties of materials, so their behavior must be well characterized to accurately predict material performance.



Pd
Pd with ^{3}He in O_h hole
^{3}He at lattice site
^{1}H

Figure 1. Tritium decays to ^{3}He without destruction to the lattice, which then becomes mobile and is trapped at vacancies. ^{3}He forms clusters which form bubbles that grow in volume.

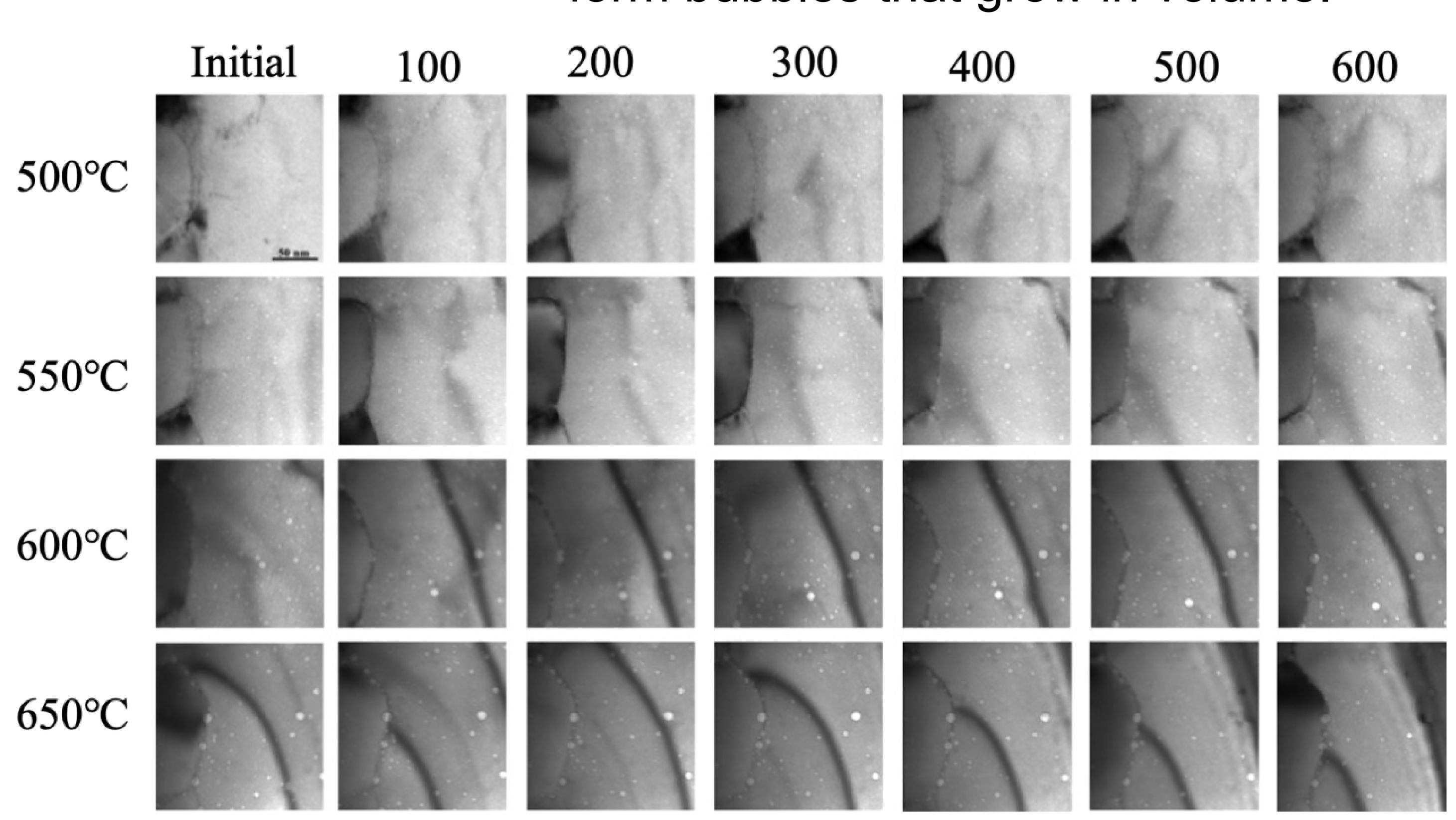


Figure 2. Summarized dataset from in-situ experiment

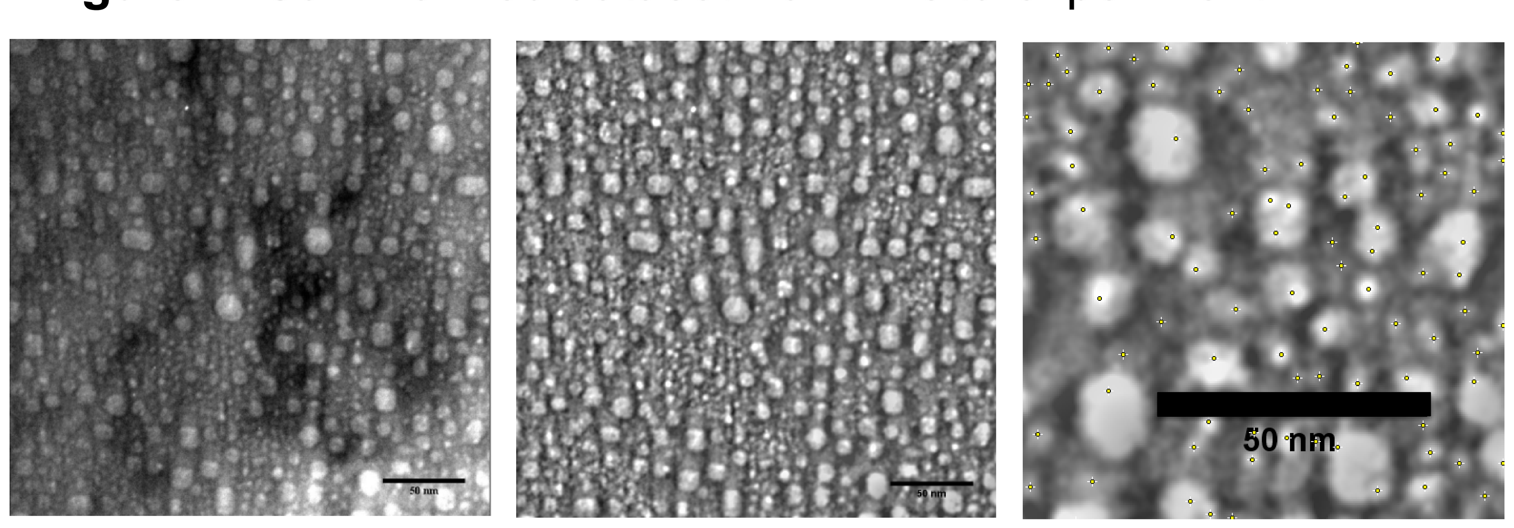


Figure 3. Image analysis process flow. First, a Gaussian Blur is applied to the image, then an FFT bandpass filter, followed by a normalized contrast to the image to increase the intensity variation between the bubbles and the background.

Out with the old, in with the new!

Results: Deep Learning Model Logistics

Problem Statement:

Can we generate an automated workflow to track the characteristics of He bubbles, and used post-processing of probability maps to unveil the underlying physics at the nanoscale?

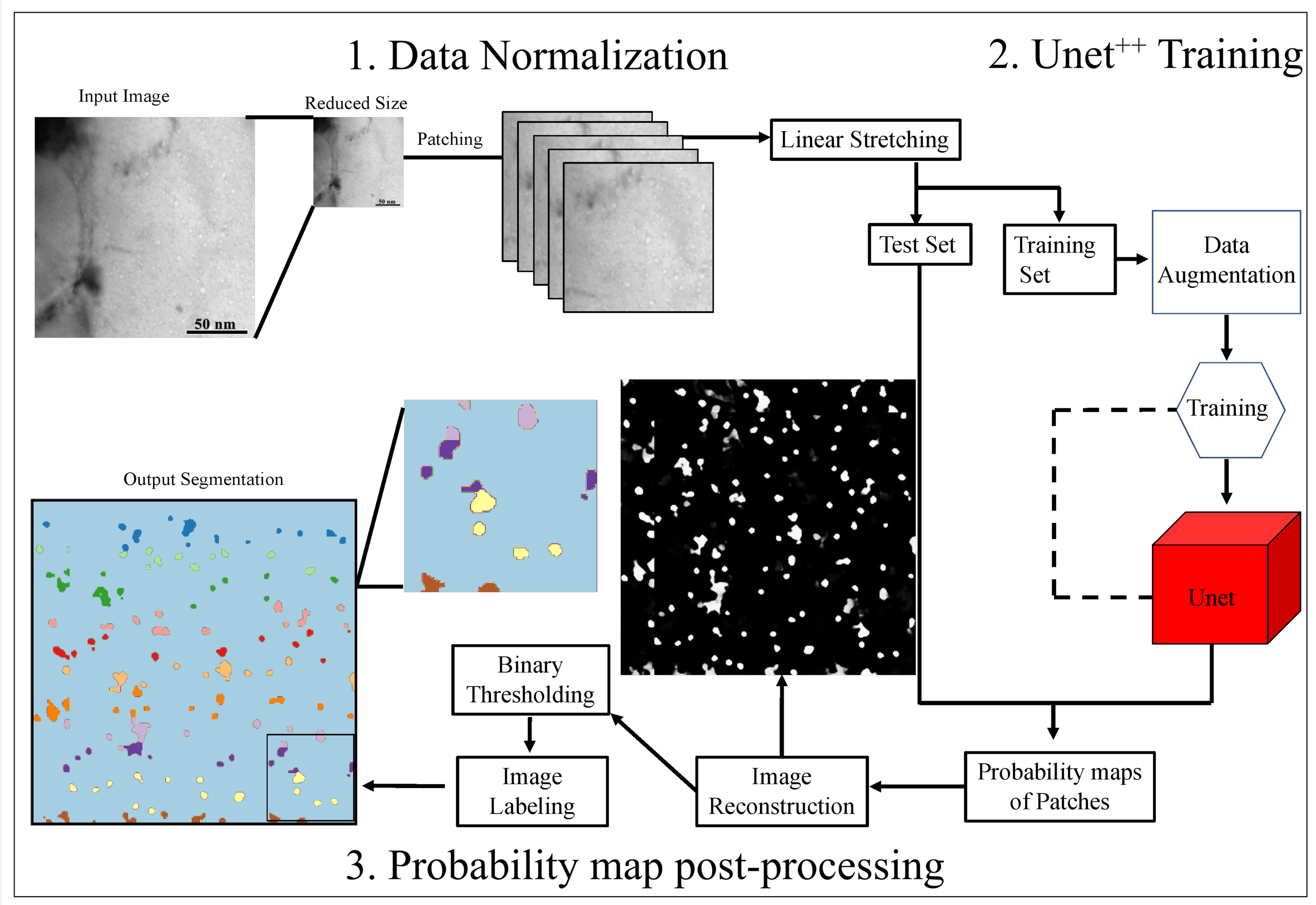


Figure 4. Diagram of the workflow dedicated to the detection and segmentation of He bubbles in Pd metal during in-situ thermal annealing of transmission electron microscopy images.

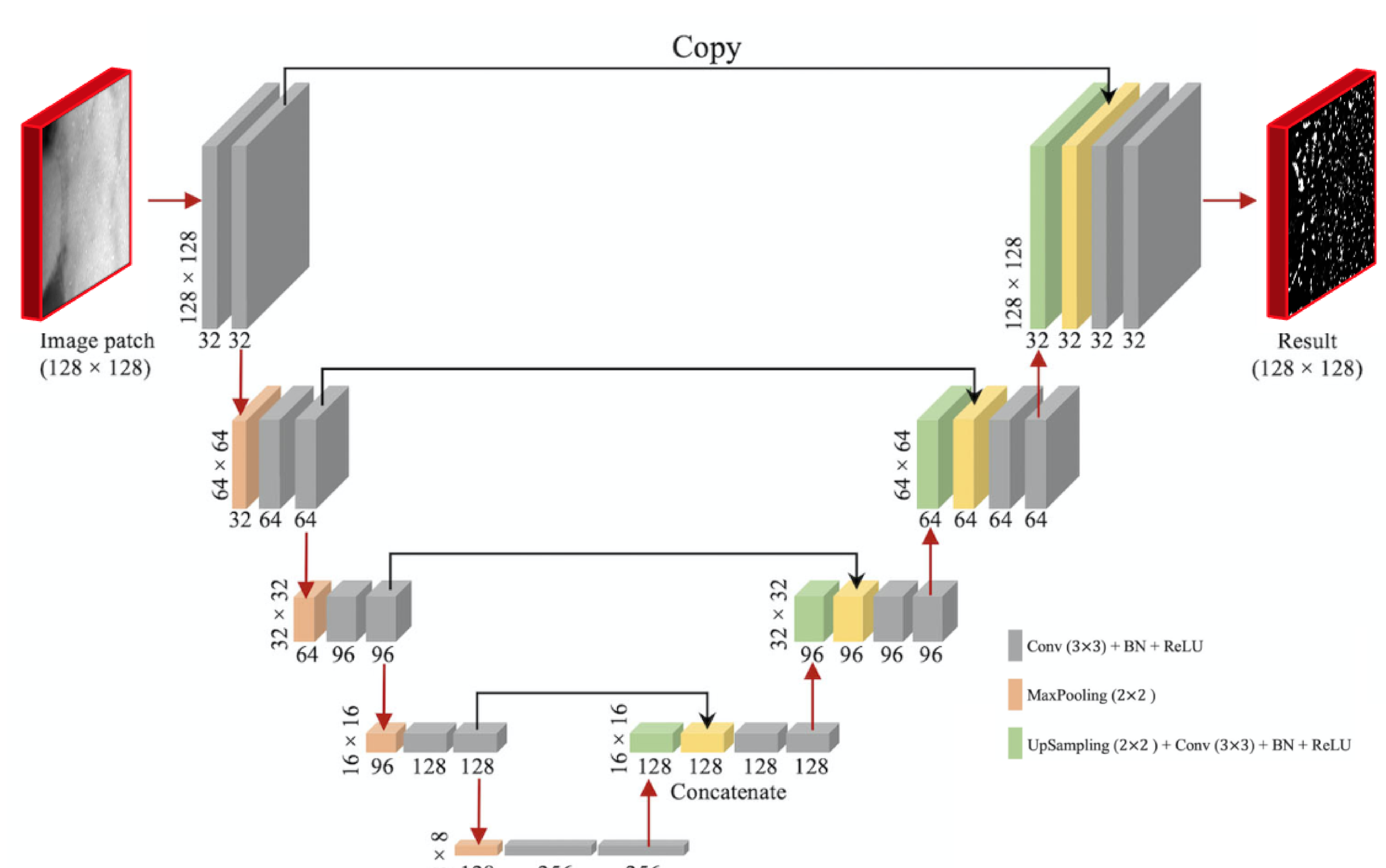


Figure 5. U-Net architecture. Boxes represent cross-sections of square feature maps. Individual map dimensions indicated on left, and number of channels indicated below dimensions. The leftmost map is a 128 × 128 normalized Pd micrograph patched from the original unfiltered image, and the rightmost represents the binary mask prediction. Red arrows represent operations, specified by the colored box, while grey arrows represent copying skip connections.

nderstanding Physics at the Nanosca

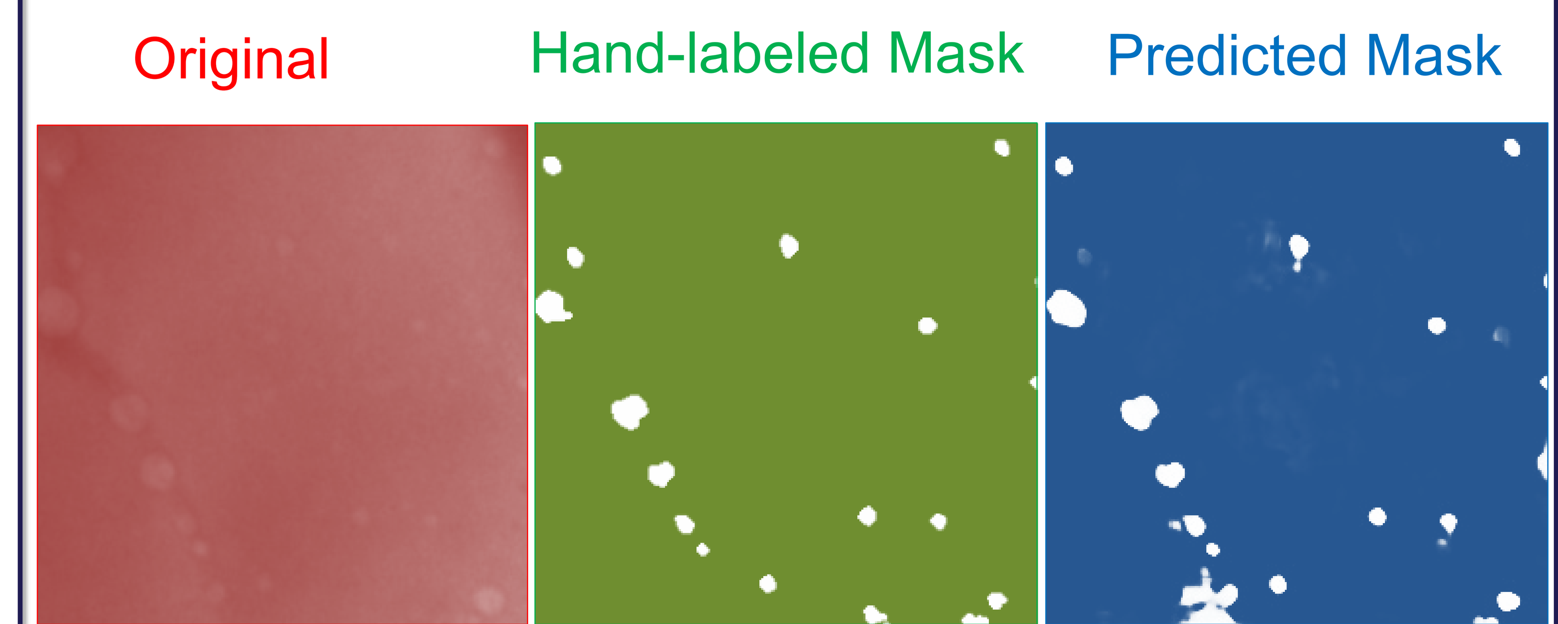


Figure 6. Patching of micrographs at grain boundaries (GB). Accuracy metrics calculated using intersection over union (IoU) of predicted mask over the hand-labeled mask. Here, we isolate GB and understand bubble features at the GB.

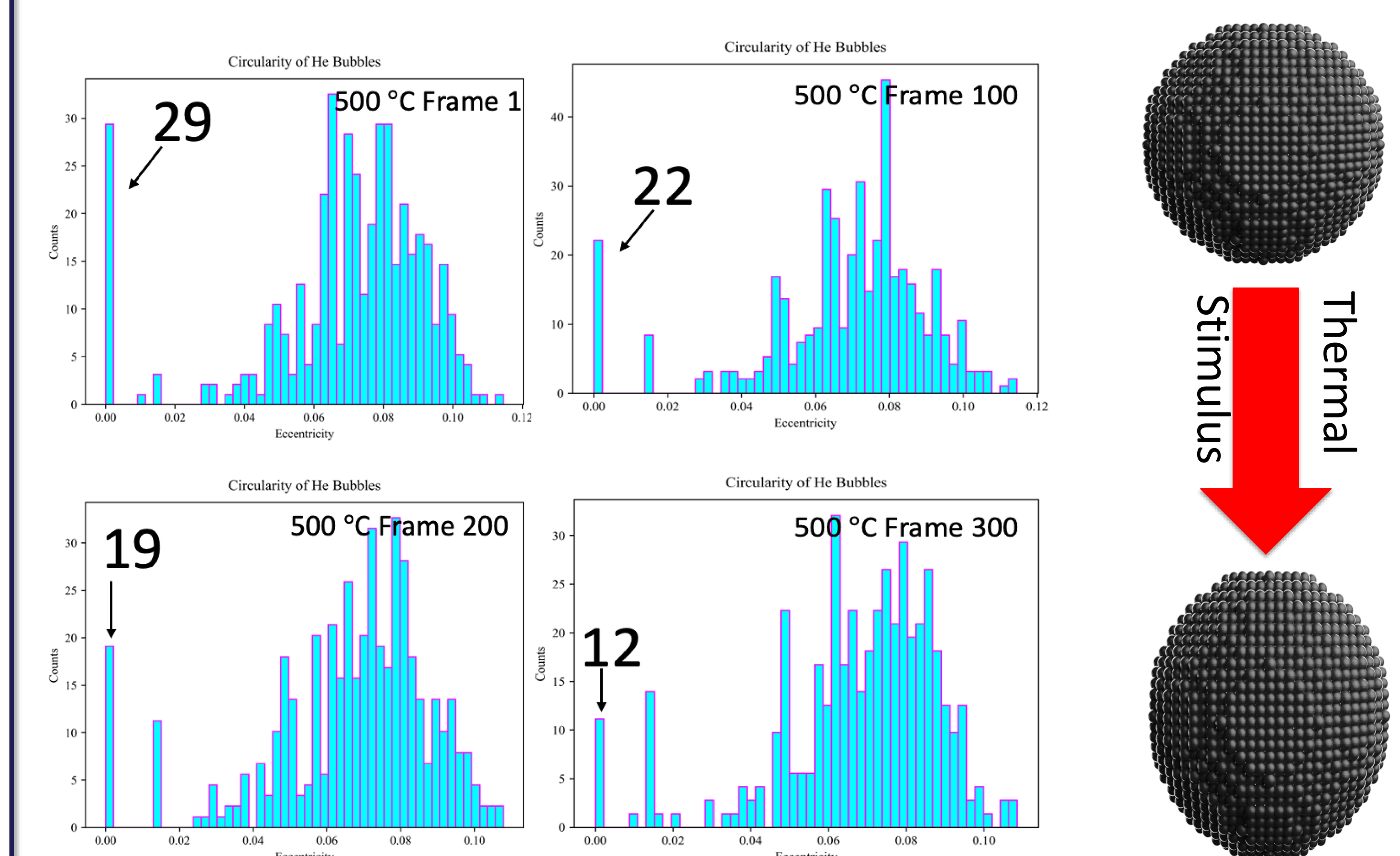


Figure 7. Histograms of He bubbles in fully reconstructed output image. Small He bubbles were perfect circles (eccentricity=0) but decrease during thermal annealing as bubble coalescence dominates in non-equilibrium processes.

Key Outcomes and Future Direction:

- New process flow serve as one of the pioneers for a new characterization paradigm for in-situ TEM
- He Bubbles migrate to grain boundaries under thermal stresses, while deformation field simultaneously distort their morphology
- Coordinate tracking allows us to expand our binary classification problem to a multi-class classification problem, yielding insights of the characteristics to individual bubbles.
- Going forward, we will expand this methodology to multiple datasets for coupled extreme environments during in situ TEM. Overall, this allows us to undergo comprehensive analyses and accelerate our understanding of physics at the nanoscale!

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