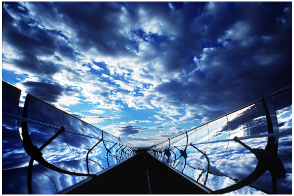
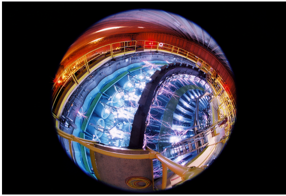
National Laboratories

SAND2021-2522C





Microstructure reconstruction via non-local patch-based image inpainting

TMS 2021 Annual Meeting & Exhibition
Anh Tran (SNL/NM), Hoang Tran (ORNL)

3/4/21

Acknowledgment

- Joint work with Hoang Tran (ORNL)
- Anh Tran and Hoang Tran. "Data-driven high-fidelity 2D microstructure reconstruction via non-local patch-based image inpainting". In: *Acta Materialia* 178 (2019), pp. 207–218. ISSN: 1359-6454

Prelude – Notation setup

- $\mathcal{D}$: unoccluded region, $\mathcal{H}$: occluded region, $\mathcal{D} \cup \mathcal{H} = \Omega$, $\mathcal{D} \cap \mathcal{H} = \emptyset$; $u : \Omega \mapsto \mathbb{R}^3$: image
- patch neighborhood $\mathcal{N}_p$, $\#\mathcal{N}_p = N$; $W_p = (u(p_1), u(p_2), \cdots, u(p_N))$
- shift map $\phi : \Omega \mapsto \mathbb{N}^2$: 2-dimensional vector field locating the nearest neighbor of a patch
- $d(W_p, W_{q'})$ – distance between 2 patches
- W_q is the nearest neighbor of W_p, which contains no occluded pixels, i.e. $q = \operatorname{argmin}_{q' \in \tilde{\mathcal{D}}} d^2(W_p, W_{q'})$
- by definition, $\phi(p) = q - p \Leftrightarrow q = p + \phi(p)$ and the nearest neighbor of W_p is $W_q = W_{p+\phi(p)}$

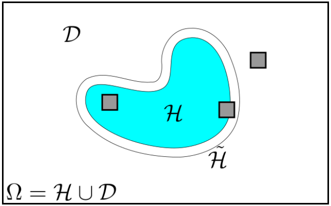


Figure: Inpainting schematic.

Pseudocode

Goal: minimize E

$$E(u, \phi) = \sum_{p \in \mathcal{H}} d^2(W_p, W_{p+\phi(p)}), \tag{1}$$

where the distance b/w patches = Euclidean distance (L^2) plus weighted L^2 derivative,

$$d^2(W_p, W_q) = \frac{1}{N} \sum_{r \in \mathcal{N}_p} \left[\| u(r) - u(r+q-p) \|_2^2 + \lambda \, \| T(r) - T(r+q-p) \|_2^2 \right]. \tag{2}$$

Approach: iterative alternating optimization, as optimizing $E(\cdot, \cdot)$ is high-dimensional and NP-hard.
Weighted mean scheme:

$$u(p) = \frac{\sum_{q \in \mathcal{N}_p} s_q^p u(p + \phi(q))}{\sum_{q \in \mathcal{N}_p} s_q^p}, \ \forall p \in \mathcal{H}, \quad s_q^p = \exp(-d^2(W_q, W_{q+\phi(q)})/(2\sigma^2)). \tag{3}$$

Algorithm 1 Minimization of $E(u, \phi)$ via iterated alternating approach.

Input: Initial guess u_0 and tolerance $\tau > 0$
Output: Inpainted image u_{k+1}

1: **repeat**
2: $\phi_k \leftarrow \operatorname{argmin}_\phi E(u^k, \phi)$ `// Nearest neighbor search (Alg 2)`
3: $u_{k+1} \leftarrow \operatorname{argmin}_u E(u, \phi^k)$ `// Image reconstruction ((3))`
4: $k \leftarrow k + 1$
5: **until** $\|u_{k+1} - u_k\| < \tau$

PatchMatch algorithm

Algorithm 2 Approximate nearest neighbor (ANN) search via PatchMatch(Barnes et al.; Fedorov, Facciolo, and Arias).

Input: Current image u, occlusion $\mathcal{H}$, number of iteration J
Output: Shift map ϕ

$\phi \leftarrow$ randomly initialize the shift map
$(p_n),\ n = 1, \ldots, |\mathcal{H}| \leftarrow$ lexicography ordering of the pixels in $\mathcal{H}$
for $j = 1, \ldots, J$ **do**
  for $n = 1, \ldots, |\mathcal{H}|$ **do**
    if j is even **then**
      $p \leftarrow p_n$ // visit the occluded pixels by lexicography order
      $a \leftarrow p - (0,1),\quad b \leftarrow p - (1,0)$ // check adjacent (up and left) pixels
    else
      $p \leftarrow p_{|\mathcal{H}|-n+1}$ // visit the occluded pixels by inverse order
      $a \leftarrow p + (0,1),\quad b \leftarrow p + (1,0)$ // check down and right pixels
    end if
    $q \leftarrow \mathrm{argmin}_{r \in \{p,a,b\}}\, d(W_p, W_{p+\phi(r)})$ // update candidate for NNs of current pixel
    $\phi(p) \leftarrow \phi(q)$
    // Random search for better NNs around the current one
    $\mathbb{S} \leftarrow$ Generate set of random 2D vectors around $\phi(p)$
    $t \leftarrow \mathrm{argmin}_{r \in \mathbb{S} \cup \{\phi(p)\}}\, d(W_p, W_{p+r})$
    $\phi(p) \leftarrow t$
  end for
end for

Multiscale scheme

Algorithm 3 Multiscale scheme (Arias et al.; Fedorov, Facciolo, and Arias; Liu and Caselles; Newson et al.)

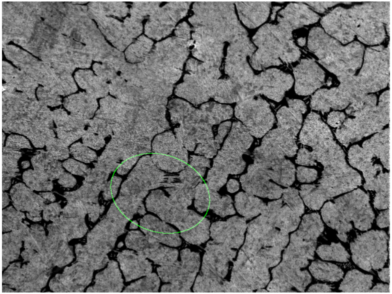
Input: known image u, occlusion $\mathcal{H}$, number of scales L
Output: inpainted image

$\{u^l\}_{l=1}^L \leftarrow$ Initialize pyramid of images (L scales) from u and $\mathcal{H}$ (coarsest scale: $l = L$);
$\{\mathcal{H}^l\}_{l=1}^L \leftarrow$ Compute pyramid of domains (L scales) from $\mathcal{H}$;
$\phi^L \leftarrow$ Random;
$u^L \leftarrow$ Initialize from ϕ^L via weighted mean scheme (3);
for $l = L, \ldots, 1$ **do**
    repeat
        $\phi^l \leftarrow$ ANN search with input $(u^l, \mathcal{H}^l)$
        $u^l \leftarrow$ Reconstruction from ϕ^l via (3)
    until converge
    $\phi^{l-1} \leftarrow$ Upsample ϕ^l
    $u^{l-1} \leftarrow$ Reconstruction from ϕ^{l-1} via (3)
end for

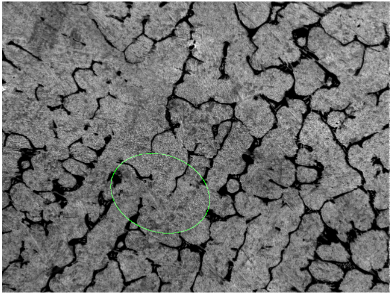
Inpainting workflow

- all images used are from UHCSDB dataset Brian L DeCost et al. “UHCSDB: UltraHigh carbon steel micrograph database”. In: *Integrating Materials and Manufacturing Innovation* 6.2 (2017), pp. 197–205
- given a random image, throw in a random occluded region (e.g. green ellipse with random sizes and orientations)
- inpaint the SEM image
- "interpolate" microstructure images

Inpainting: examples and results 1/8

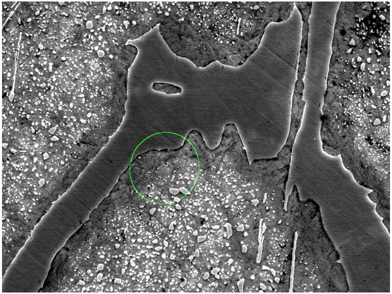


(a) Orig. #35.

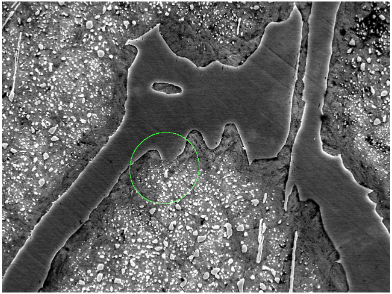


(b) Recon. #35.

Inpainting: examples and results 2/8

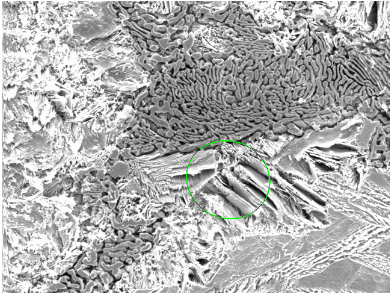


(a) Orig. #1098.

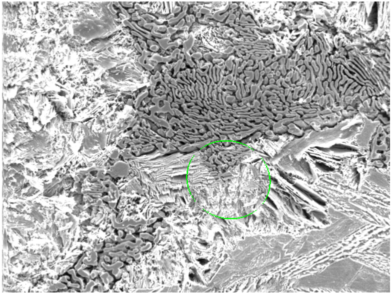


(b) Recon. #1098.

Inpainting: examples and results 3/8

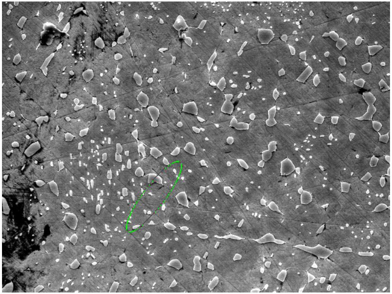


(a) Orig. #1294.

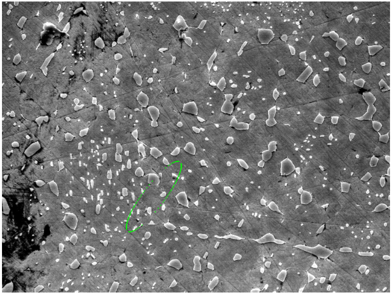


(b) Recon. #1294.

Inpainting: examples and results 4/8

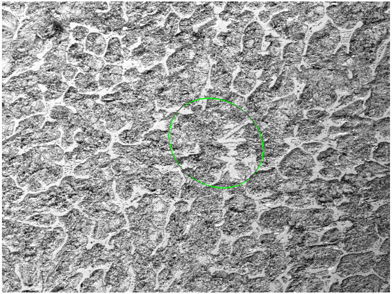


(a) Orig. #1633.

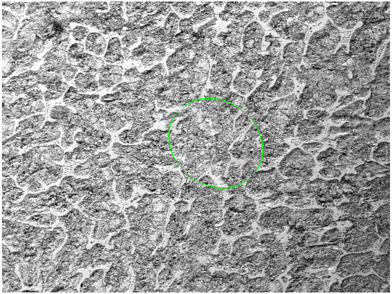


(b) Recon. #1633.

Inpainting: examples and results 5/8

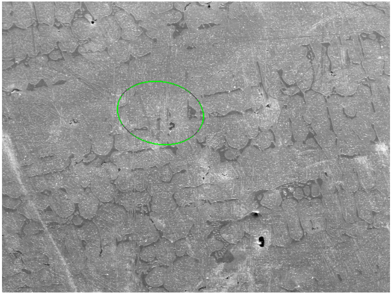


(a) Orig. #1718.

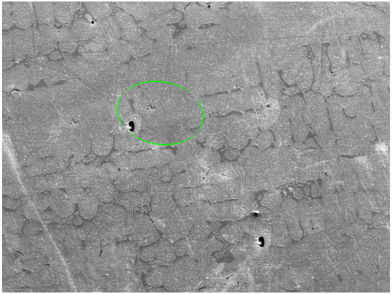


(b) Recon. #1718.

Inpainting: examples and results 6/8

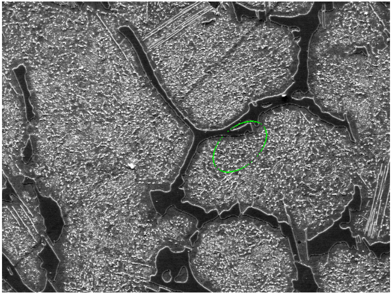


(a) Orig. #1561.

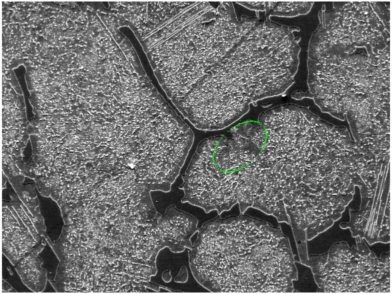


(b) Recon. #1561.

Inpainting: examples and results 7/8

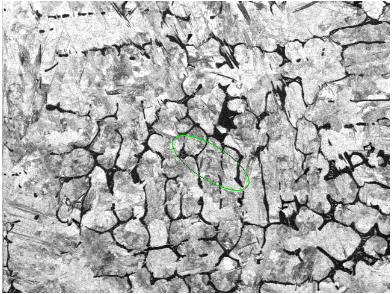


(a) Orig. #1457.

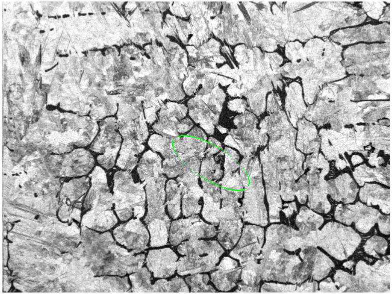


(b) Recon. #1457.

Inpainting: examples and results 8/8



(a) Orig. #36.

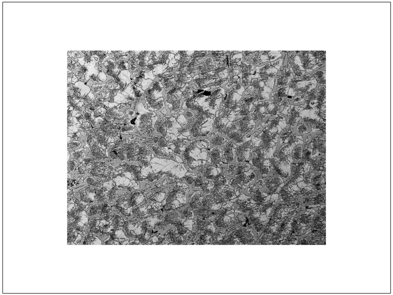


(b) Recon. #36.

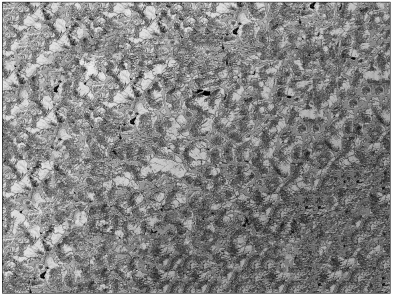
Outpainting workflow

- all images used are from UHCSDB dataset Brian L DeCost et al. "UHCSDB: UltraHigh carbon steel micrograph database". In: *Integrating Materials and Manufacturing Innovation* 6.2 (2017), pp. 197–205
- try to "extrapolate" beyond the given images
- results vary depending on how many features are available
- "busier" images tend to yield better results

Outpainting: examples and results 1/9

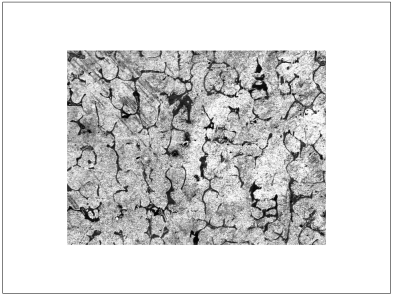


(a) Orig. #1552.

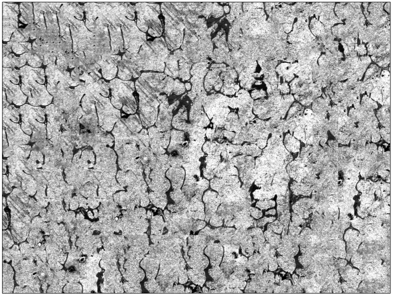


(b) Recon. #1552.

Outpainting: examples and results 2/9

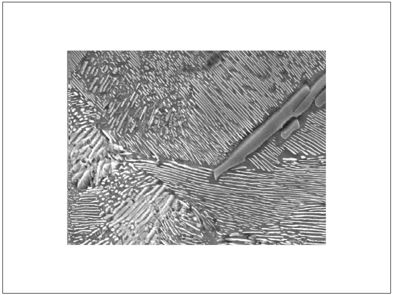


(a) Orig. #1583.

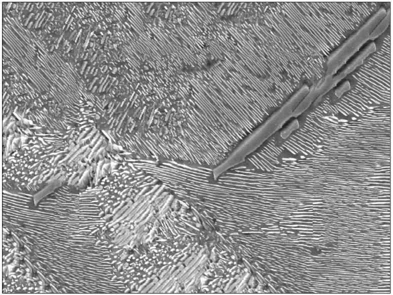


(b) Recon. #1583.

Outpainting: examples and results 3/9

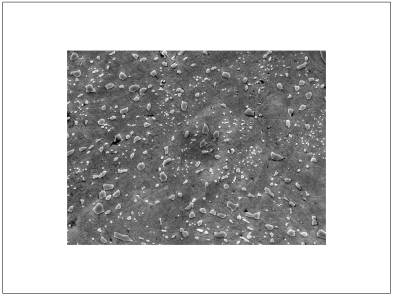


(a) Orig. #1597.

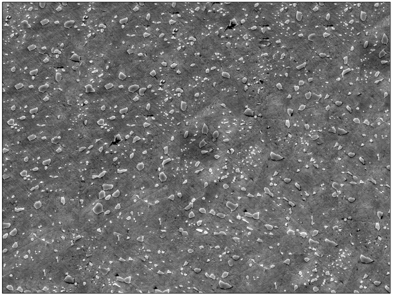


(b) Recon. #1597.

Outpainting: examples and results 4/9



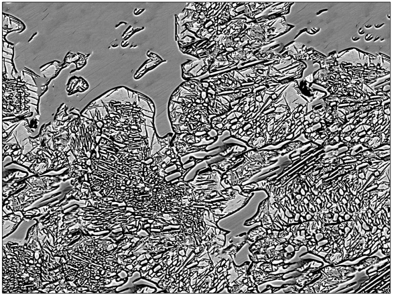
(a) Orig. #1676.



(b) Recon. #1676.

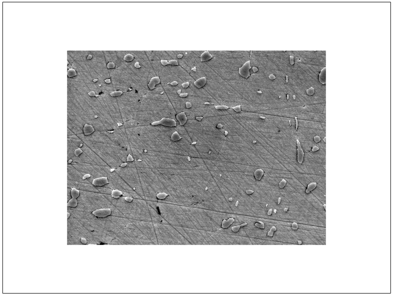
Outpainting: examples and results 5/9

(a) Orig. #1531.



(b) Recon. #1531.

Outpainting: examples and results 6/9



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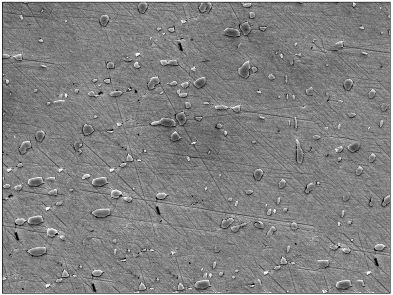
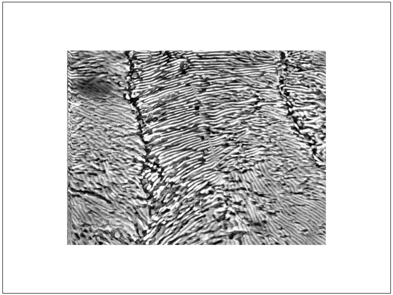
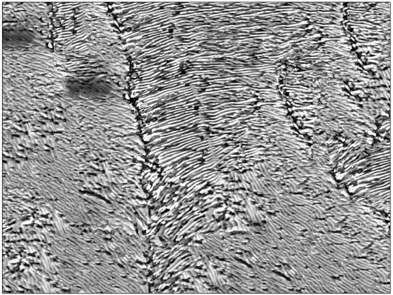


(b) Recon. #1569.

Outpainting: examples and results 7/9

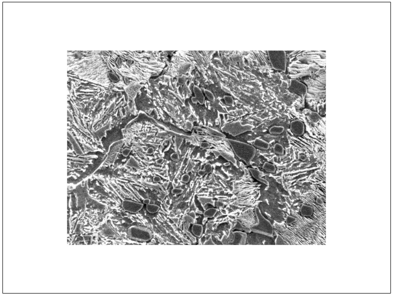


(a) Orig. #1589.

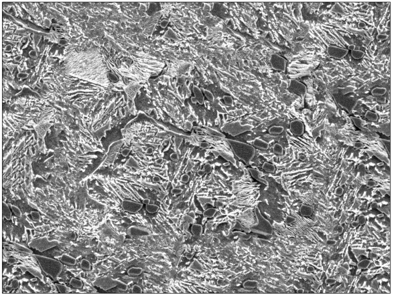


(b) Recon. #1589.

Outpainting: examples and results 8/9

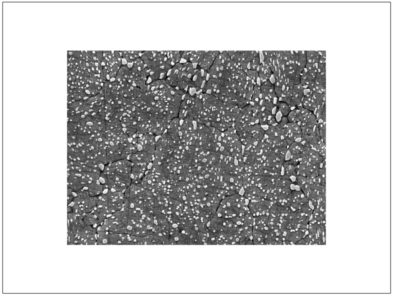


(a) Orig. #1656.

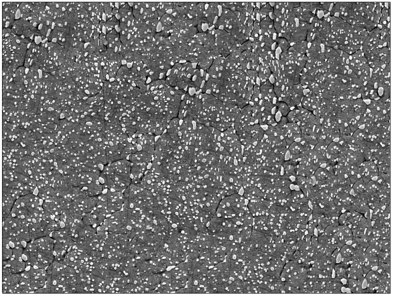


(b) Recon. #1656.

Outpainting: examples and results 9/9



(a) Orig. #1694.



(b) Recon. #1694.

Stitching images – or microstructure assembly

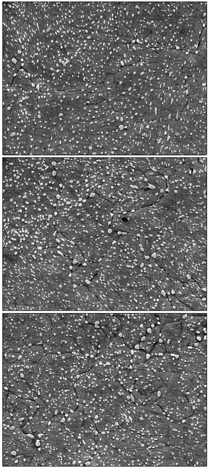
- context: many microstructure images taken at **different locations** for the **same** specimen – supposed to be **statistically equivalent** by definition
- **question**: given a set of finitely many images, can we reconstruct the microstructure of the **whole** specimen?
- an example of shuffling and $\rightarrow$ $\mathbf{n!}$ synthetic big SEM microstructure images

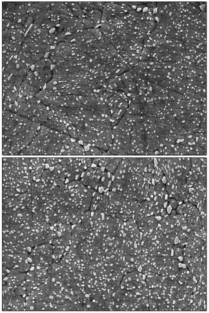
SEM 1		SEM 2
	SEM 3	
SEM 4		SEM 5

SEM 5		SEM 4
	SEM 3	
SEM 2		SEM 1

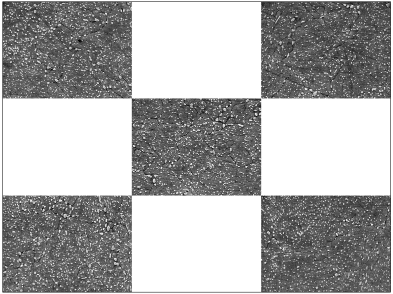
Stitching images

- all images used are from UHCSDB dataset Brian L DeCost et al. "UHCSDB: UltraHigh carbon steel micrograph database". In: *Integrating Materials and Manufacturing Innovation* 6.2 (2017), pp. 197–205
- *primary_microconstituent = spheroidite*
- 970°C for 5 minutes before quenched
- label AC1_970C_5M_Q
- #272, #1013, #596, #1094, #286
- **same** magnification 4910X

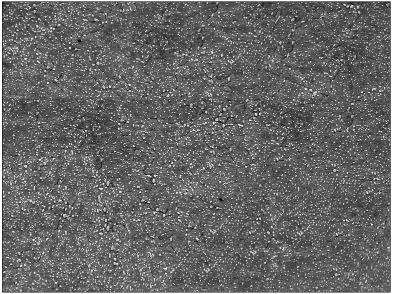




Stitching: examples and results 1/6

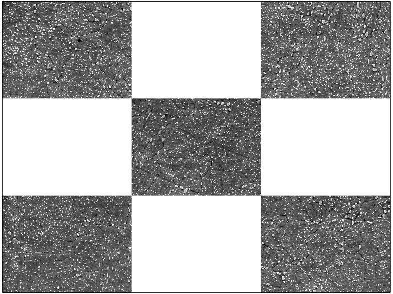


(a) Input #11/120.

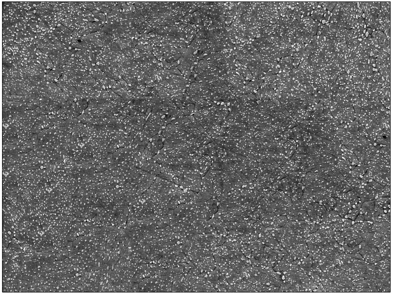


(b) Recon. #11/120.

Stitching: examples and results 2/6

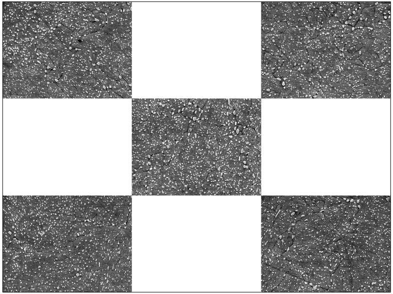


(a) Input #13/120.

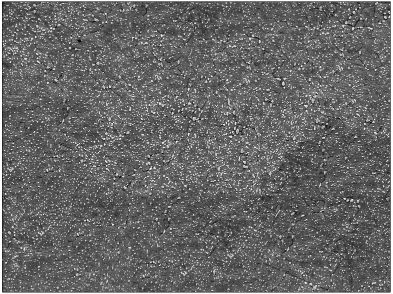


(b) Recon. #13/120.

Stitching: examples and results 3/6

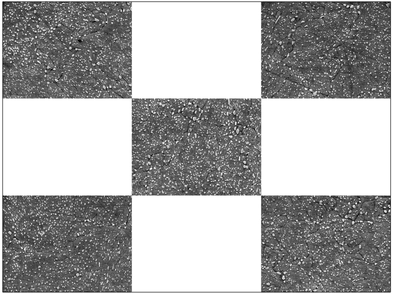


(a) Input #18/120.

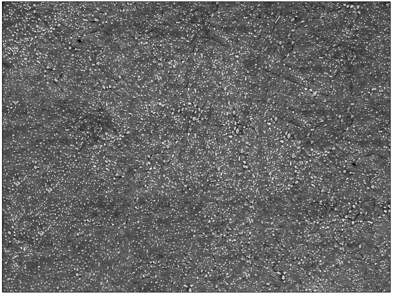


(b) Recon. #18/120.

Stitching: examples and results 4/6

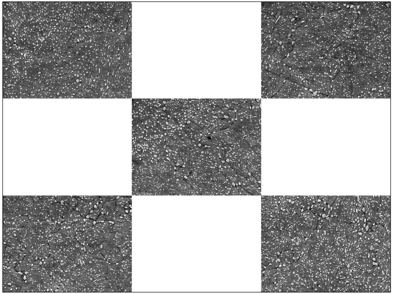


(a) Input #19/120.

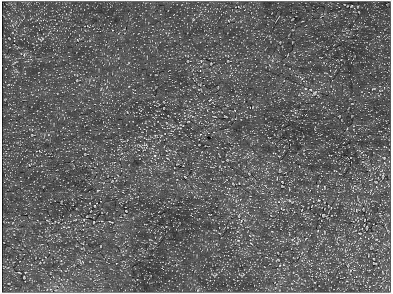


(b) Recon. #19/120.

Stitching: examples and results 5/6

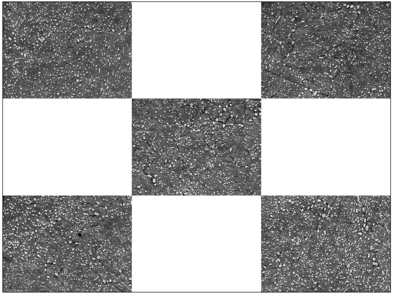


(a) Input #24/120.

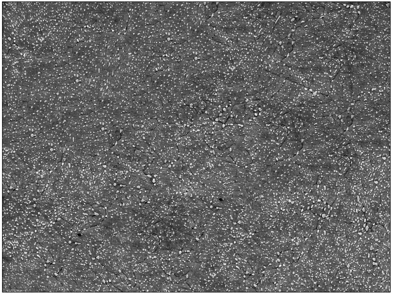


(b) Recon. #24/120.

Stitching: examples and results 6/6



(a) Input #30/120.



(b) Recon. #30/120.

Conclusion

This talk is about

- an extended image inpainting method
- applied for microstructure
  - inpainting
  - outpainting
  - "assembly" – stitching images (of the same magnification) at different places
- mostly limited to single-image; does not generalize to multi-image (as opposed to GAN)
- might be useful to go from Small Data to Big Data

Thank you for listening.

Q/A.

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