Physics-Based Super-Resolution for Electron Backscatter Diffraction (EBSD)

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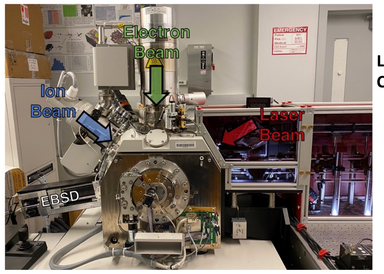
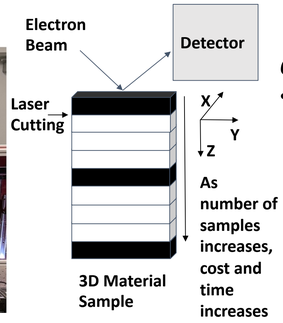
Award #1934641 and #1664172 GitHub Link

Introduction



TriBeam Experiment



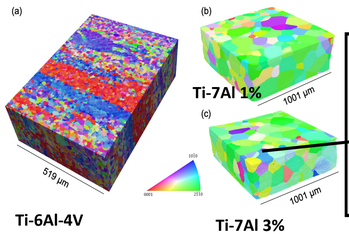
3D Data Collection

Objective:

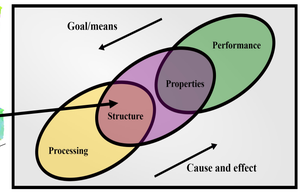
- Generate high-resolution EBSD microstructure given sparsely sampled EBSD microstructure (collected by TriBeam experiment)

TriBeam Experiment:

- Collect EBSD Microstructures: Ordered arrangement of crystals
- EBSD: Orientation information of crystal at each voxel
- PSP is a guiding principle in materials design and development



EBSD Microstructures

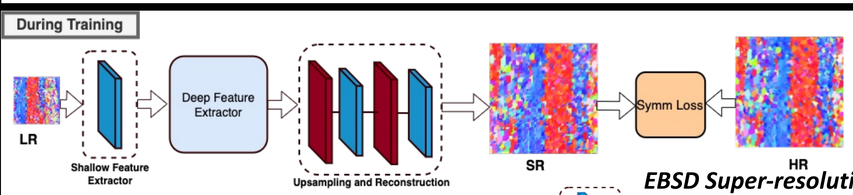


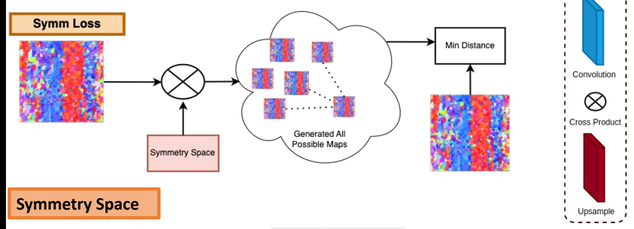
Process-Structure-Properties (PSP)
Ref: msestudent.com/what-is-materials-science-tetrahedron-paradigm

Challenges with Experimental Microstructure:

- ***Time Consuming:*** 6 months to collect and reconstruct Ti64 microstructure of sample size 740 X 519 X 213 (micrometer)
- ***Cost:*** Tens of thousands of dollars per week to run experiments
- ***Expensive Equipment :*** Experiment setup (Tri-beam) available only at three places in whole North America

Method



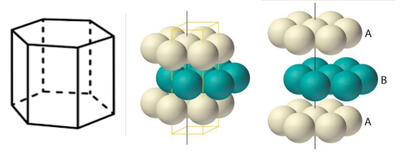


EBSD Super-resolution (EBSD-SR):

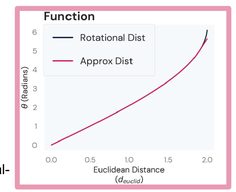
- Network trained is in quaternion orientation domain
- Symmetries and distances can be defined and calculated easily in quaternion domain
- Approximate rotational distance with symmetry is our physics-based loss
- Physics-based loss is inspired from crystallography
- Incorporate HCP symmetry information in loss function
- All generated output are reduced to fundamental zone during inference

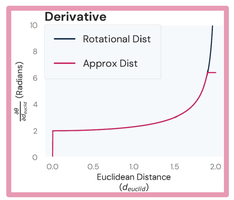
Rotational Distance Loss:

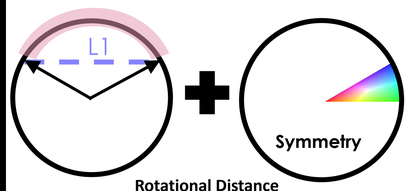
$$\theta = 2\cos^{-1}\left(Re(q_1 q_2^*)\right)$$
$$= 2\cos^{-1}\left(<\vec{q_1}, \vec{q_2}>\right)$$
$$= 2\cos^{-1}\left(1 - \frac{1}{2}\|\vec{q_1} - \vec{q_2}\|_2^2\right)$$
$$= 4\sin^{-1}\left(\frac{1}{2}\|\vec{q_1} - \vec{q_2}\|_2\right)$$
$$\theta = 4\sin^{-1}\left(\frac{d_{\text{euclid}}}{2}\right) \quad \text{where, } d_{\text{euclid}} = \|q_1 - q_2\|_2.$$



Hexagonal Closed Pack (HCP) Structure
Ref:https://2012books.lardbucket.org/books/principles-of-general-chemistry-v1.0/s16-02-the-arrangement-of-atoms-in-cr.html



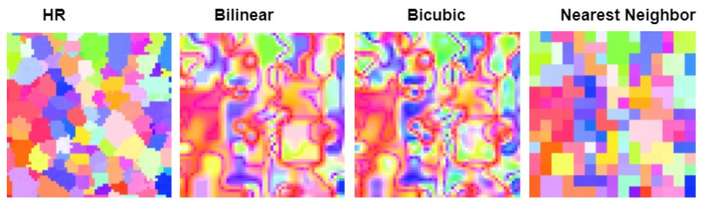




Rotational Distance

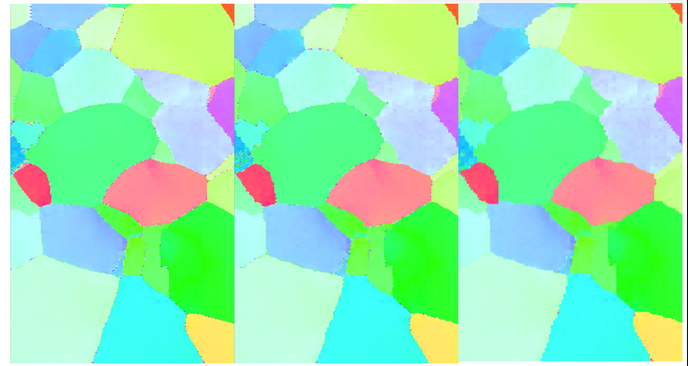
Experimental Results

Results for Ti-6Al-4V

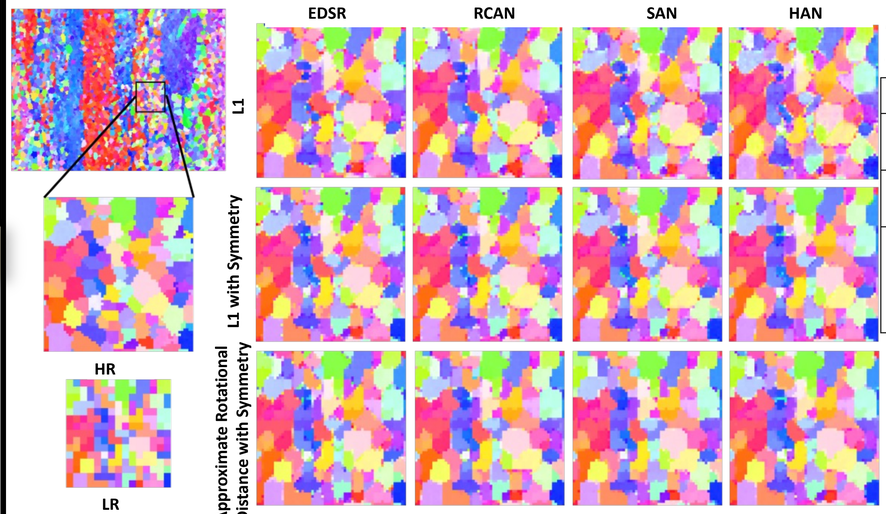


x4	Bilinear	Bicubic	Nearest Neighbor
PSNR/SSIM	11.30 / 0.237	11.22 / 0.211	**13.25 / 0.373**

Results for Ti-7Al 1%



L1 | L1 with Symmetry | Rot dist approx with Symmetry



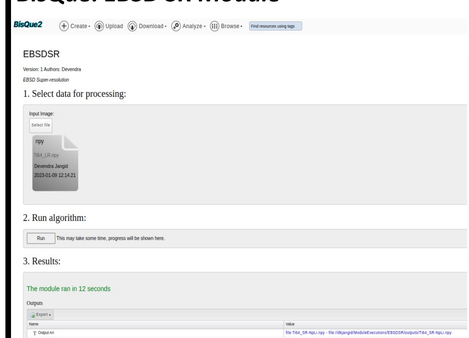
PSNR/SSIM comparison for 4x super-resolution scaling across networks, losses and materials

	EDSR	RCAN	SAN	HAN
L1 (No Physics)	14.85 / 0.472	**14.89 / 0.474**	14.83 / 0.465	14.65 / 0.450
L1 with Symm	15.05 / 0.483	15.07 / 0.484	15.04 / 0.484	**15.13 / 0.497**
Rot Dist approx. with Symm	15.02 / 0.486	15.24 / 0.509	15.23 / 0.510	**15.30 / 0.513**

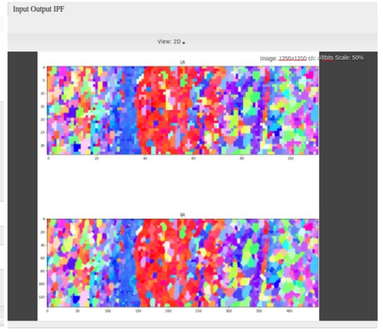
	Ti-6Al-4V	Ti-7Al 3%	Ti-7Al 1%
L1 (No Physics)	14.94/ 0.478	26.66/ 0.865	25.37/ 0.852
L1 with Symm	15.19/ 0.497	26.82/ 0.869	25.38/ 0.856
Rot Dist approx. with Symm	**15.35/ 0.5264**	**27.25/ 0.881**	**25.72/ 0.871**

BisQue

BisQue: EBSD SR Module



Visualization



- **BisQue:** A free and open-source web-based platform: https://bisque2.ece.ucsb.edu/client_service/
- Easy share of data as well as analysis
- Simple and scalable module integration system for analysis tasks over images and meta data
- Users can use EBSD SR module on BisQue
- Input is a LR EBSD in quaternion and Output is a SR EBSD in quaternion
- EBSD Data can be visualized on BisQue

Reference

Reference: Jangid, D.K., Brodnik, N.R., Goebel, M.G. *et al.* Adaptable physics-based super-resolution for electron backscatter diffraction maps. *npj Comput Mater* **8**, 255 (2022). https://doi.org/10.1038/s41524-022-00924-2

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