Supplementary Information for "A Deep Learning Approach for Complex Microstructure Inference"

by
Ali Riza Durmaz[1,2,3,*,+], Martin Müller[4,5,+] Bo Lei[6], Akhil Thomas[1,3], Dominik Britz[4,5], Elizabeth A. Holm[6], Chris Eberl[1,3], Frank Mücklich[4,5], and Peter Gumbsch[1,2]

1: Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, 79108, Germany
2: Karlsruhe Institute of Technology (KIT), Institute for Applied Materials IAM, Karlsruhe, 76131, Germany
3: University of Freiburg, Freiburg, 79110, Germany
4: Saarland University, Department of Materials Science, Saarbrücken, 66123, Germany
5: Material Engineering Center Saarland, Saarbrücken, 66123, Germany
6: Carnegie Mellon University, Department of Materials Science and Engineering, Pittsburgh, PA 15213, USA

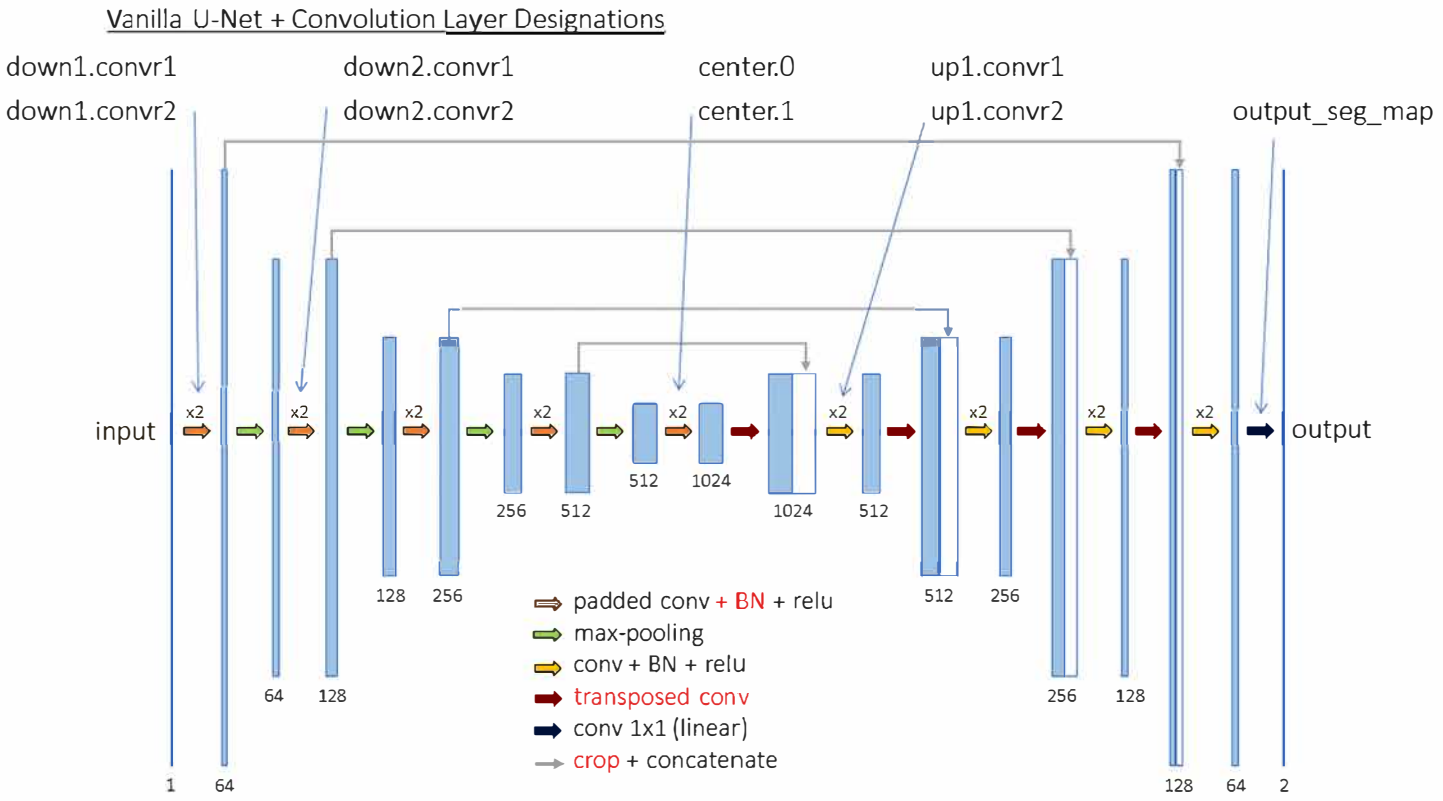
*: ali.riza.durmaz@iwm.fraunhofer.de
+: these authors contributed equally to this work

Supplementary Table 1: Number of images and their lath-shaped bainite content for each fold of each of the four data sets.

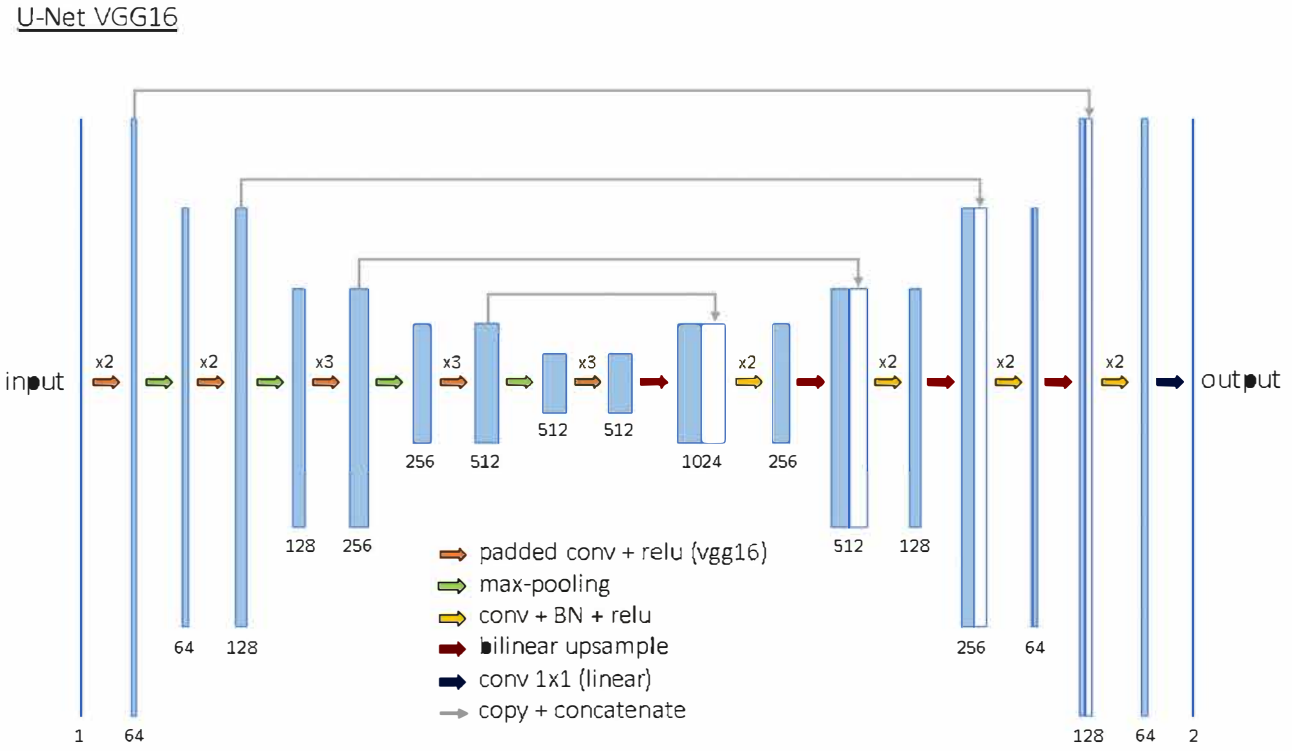
Dataset	Fold	0	1	2	3	4
LOM	Number of tile images	151	151	151	151	150
	Bainite pixel percentage [%]	27	26.3	27.4	31.2	29.8
LOM downscaled	Number of tile images	36	36	36	36	35
	Bainite pixel percentage [%]	30.6	26.7	25.2	28	25.4
SEM	Number of tile images	83	83	83	82	82
	Bainite pixel percentage [%]	50.9	58.6	62.3	63.2	60.2
SEM downscaled	Number of tile images	27	27	27	27	27
	Bainite pixel percentage [%]	50.9	46.8	55.3	55.1	59.5

Supplementary Table 2: Number of images and their lath-shaped bainite content for each fold of each of the data sets from tile experiment.

Tile size	Fold	0	1	2	3	4
64	Number of tile images	2612	2611	2611	2611	2611
	Bainite pixel percentage [%]	27.2	27.7	27.1	27.8	27.5
96	Number of tile images	1020	1020	1020	1020	1020
	Bainite pixel percentage [%]	27.0	29.7	27.7	29.3	28.1
128	Number of tile images	653	653	653	653	652
	Bainite pixel percentage [%]	27.3	27.2	27.2	28.7	26.9
192	Number of tile images	255	255	255	255	255
	Bainite pixel percentage [%]	28.4	28.5	29.0	27.3	28.7
256	Number of tile images	164	163	163	163	163
	Bainite pixel percentage [%]	25.8	28.4	27.1	28.5	27.4
512	Number of tile images	41	41	41	41	40
	Bainite pixel percentage [%]	27.6	29.0	27.4	29.1	24.1



Supplementary Figure 1: Vanilla U-Net architecture.



Supplementary Figure 2: VGG16 U-Net architecture.

Supplementary Table 3: Description of individual augmentations applied for vanilla U-Net models on LOM images.

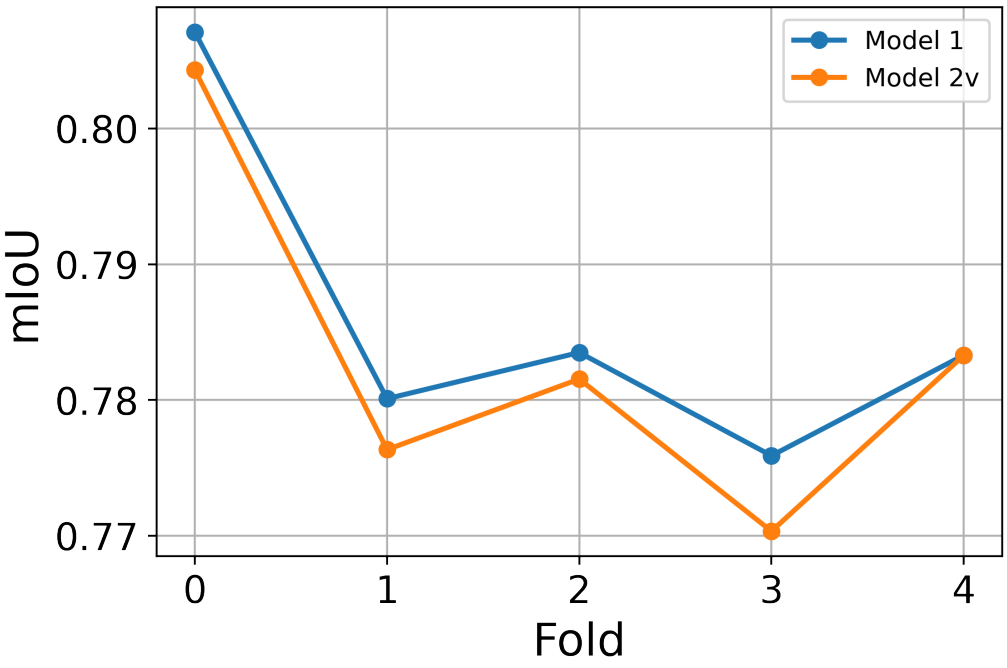
Augmentation type	Description: aug. type / parameter(s)	x_{lim}	p
Affine transformation	Linear transformation / rotate, shift and scale limit	30, 0.1, 0.1	0.8
Rotation 90 °	- / -	-	0.25
Reflection	- / -	-	0.25
Elastic transformation	Local deformations / alpha affine, alpha, sigma, approx.	0, 15.86, 5.15, True	0.35
Optical distortion	Barrel or pincushion / distort limit, shift limit	0.07, 0.23	0.25

Table 2: Description of individual augmentations applied for vanilla U-Net models on SEM images

Augmentation type	Description: aug. type / parameter(s)	x_{lim}	p
Affine transformation	Linear transformation / rotate, shift and scale limit	30, 0.1, 0.1	0.8
Rotation 90 °	- / -	-	0.25
Reflection	- / -	-	0.25
Elastic transformation	Local deformations / alpha affine, alpha, sigma, approx.	0, 40.52, 7.77, True	0.35
Optical distortion	Barrel or pincushion / distort limit, shift limit	0.14, 0.42	0.25
Gaussian blurring	Convolution Gaussian kernel / blur kernel size	9	0.2
Motion blurring	Convolution motion-blur kernel / blur kernel size	7	0.2

Supplementary Table 4: Description of augmentations applied for UNet-Vgg16 models.

Augmentation type	Description: aug. type / parameter(s)	x_{lim}	p
Affine transformation	Linear transformation / rotate, shift and scale limit	45, 0, 0.2	0.7
Reflection	- / -	-	0.5
Elastic transformation	Local deformations / alpha affine, alpha, sigma, approx.	0, 40, 6, True	0.5
Grid Distortion	Local deformations / num steps, distort limit	5, 0.2	0.5
Gaussian blurring	Convolution Gaussian kernel / blur kernel size	7	0.2
Motion blurring	Convolution motion-blur kernel / blur kernel size	5	0.2
Gaussian noise	- / var limit	(10,50)	0.2
Contrast	- / limit	0.15	0.7
Brightness	- / limit	0.1	0.7

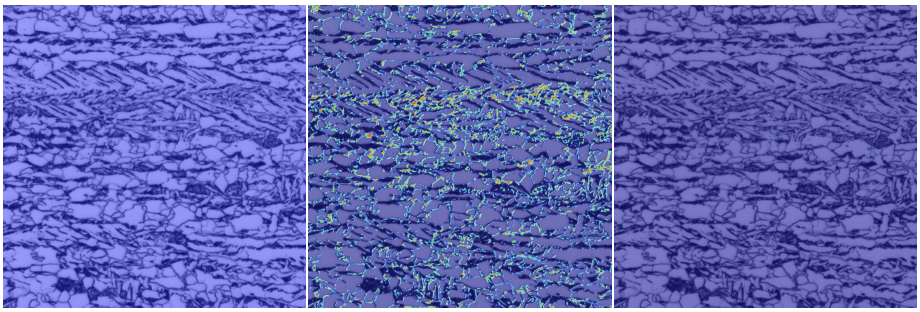


Supplementary Table 3: Class-averaged IoU for the different folds for two exemplary models.

Supplementary Table 5: Description of individual training + validation as well as testing times for both architectures in the best configurations.

	Vanilla U-Net		VGG16 U-Net	
Dataset	Train + validation	Test on full scale images	Train + validation	Test on full scale images
LOM	256×256, 8 ms/image	1024×1024, 92 ms/image	256×256, 47 ms/image	1024×1024, 240 ms/image
SEM	512×512, 134 ms/image	1024×717, 74 ms/image	512×512, 200 ms/image	1024×717, 160 ms/image

Supplementary Figure 4: Grad-CAM maps indicating image regions that dictated the decision of the Vanilla U-Net network with respect to the background class. The individual panel captions refer to the specific network layer for which the activation map is computed (see Supplemental Figure 1).



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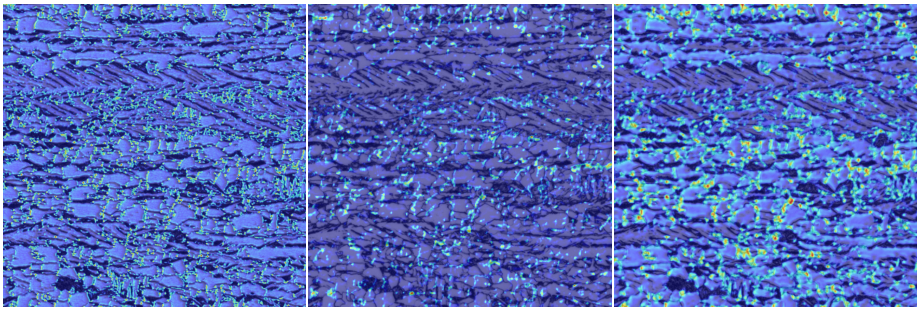

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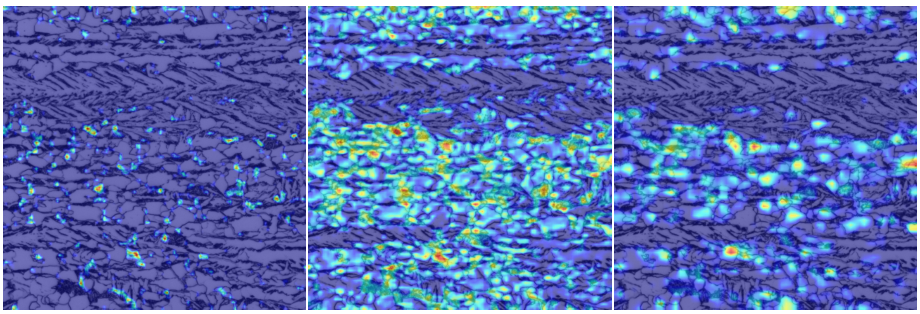
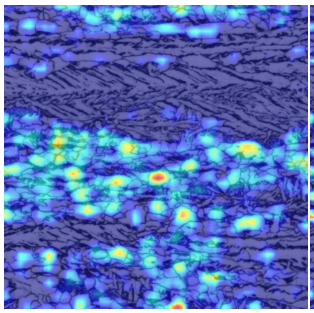
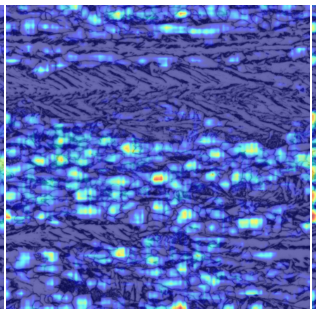


(4.7) down4.convr1 (4.8) down4.convr2 (4.9) center.0



(4.10) center.1



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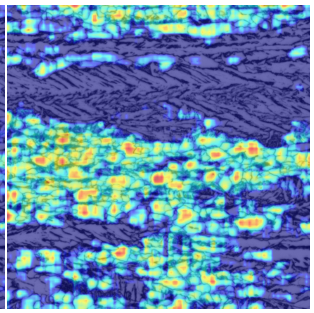

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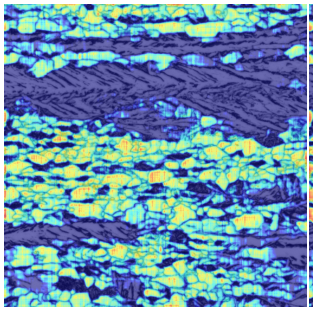

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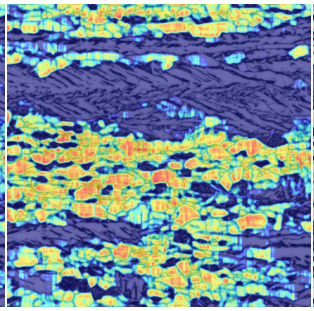

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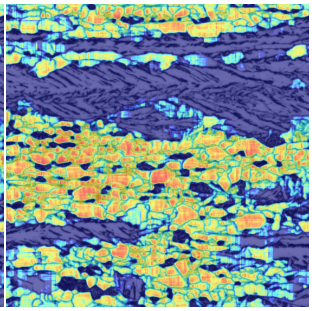

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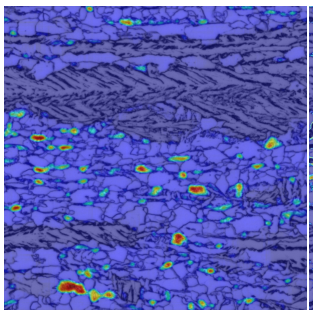

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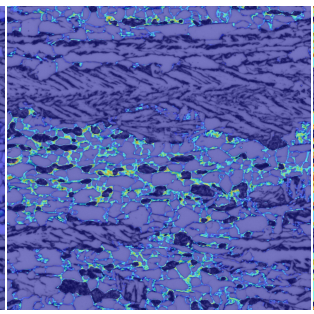

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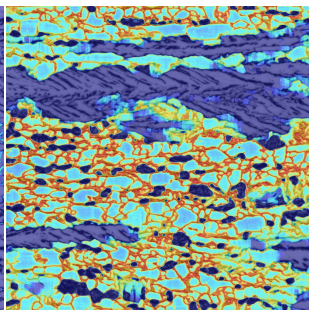

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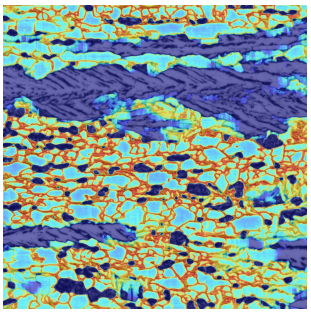
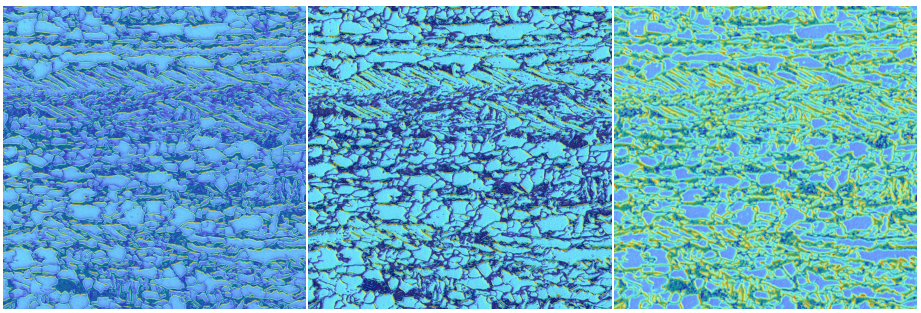


(4.19) output.seg.mask

Supplementary Figure 5: Grad-CAM maps indicating image regions that dictated the decision of the Vanilla U-Net network with respect to the foreground class. The individual panel captions refer to the specific network layer for which the activation map is computed (see Supplemental Figure 1).



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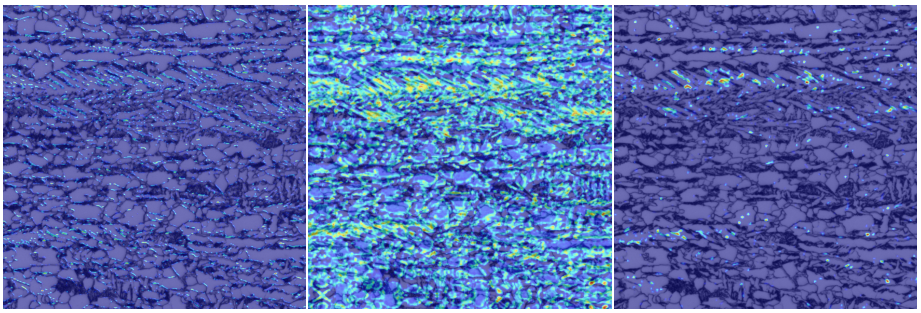

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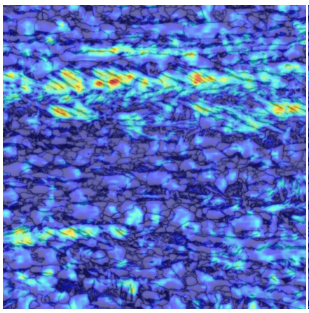
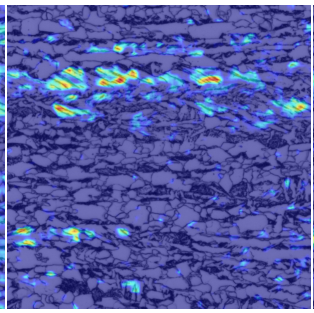
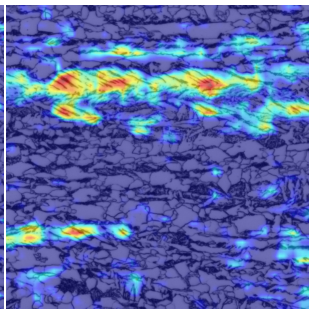


(5.7) down4.convr1



(5.8) down4.convr2



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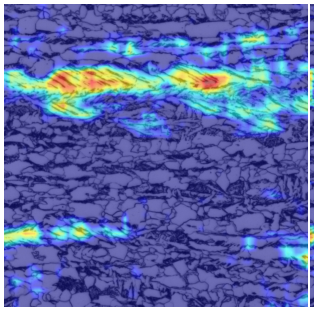

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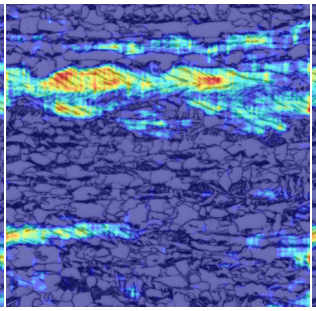
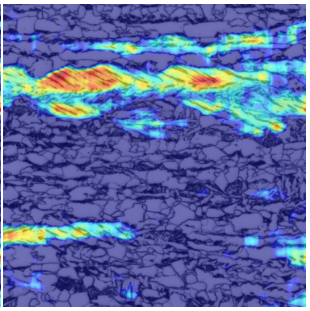
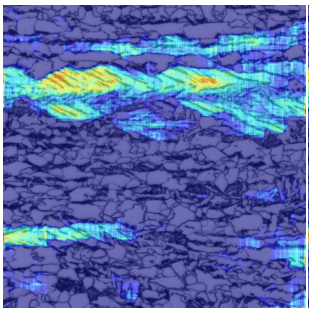


(5.11) up1.convr1



(5.12) up1.convr2



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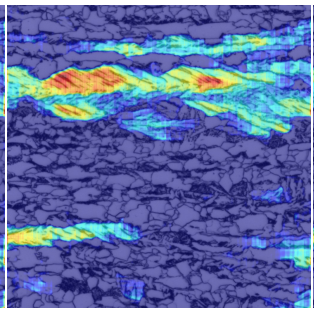

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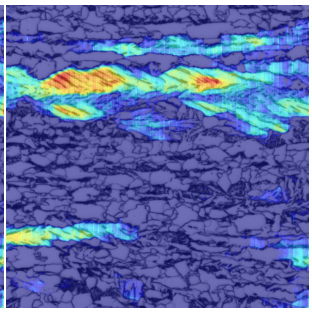

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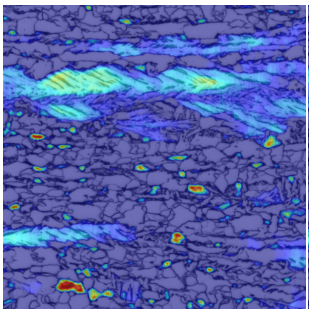

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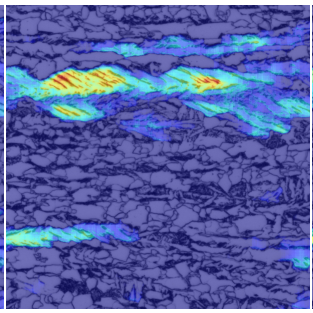

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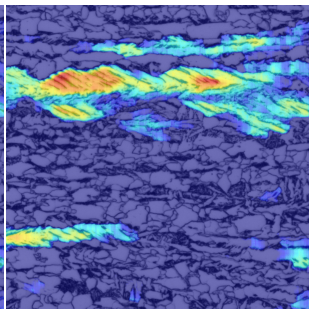

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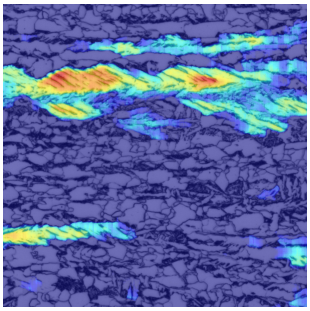
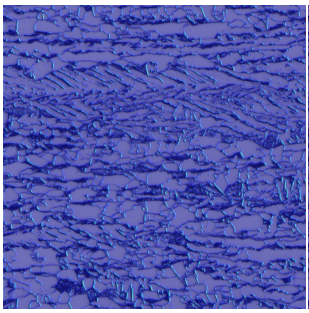
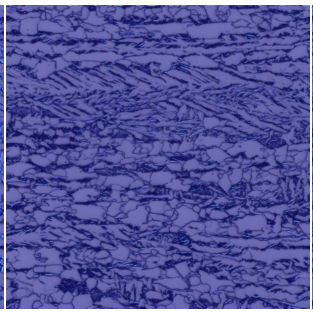


(5.19) output.seg.mask

Supplementary Figure 6: Grad-CAM maps indicating image regions that dictated the decision of the VGG U-Net network with respect to the background class. The individual panel captions refer to the specific network layer for which the activation map is computed (see Supplemental Figure 1 and 2).



(6.1) down1.convr1



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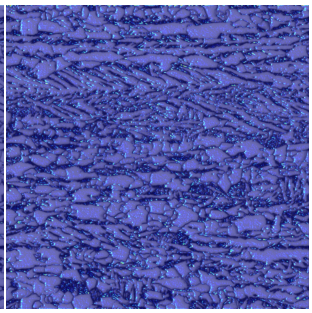
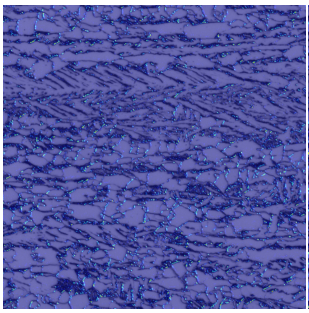


(6.3) down2.convr1



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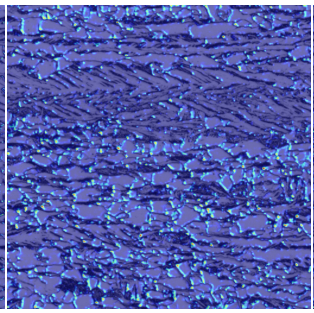

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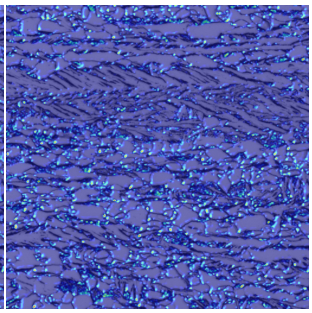
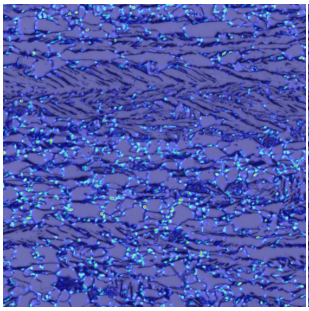


(6.6) down3.convr2



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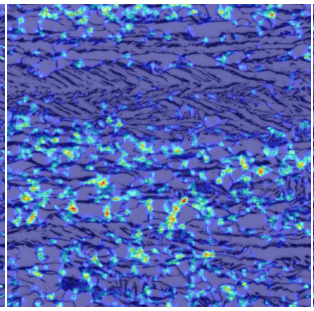
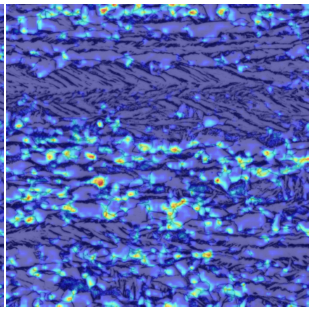
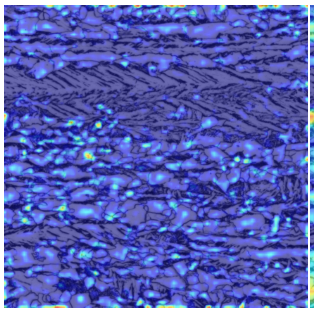


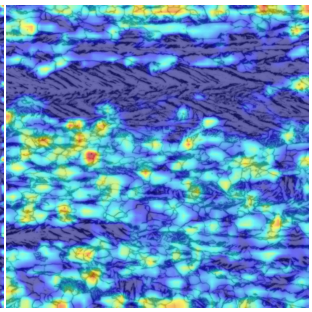
(6.8) down4.convr1



(6.9) down4.convr2



(6.10) down4.convr3



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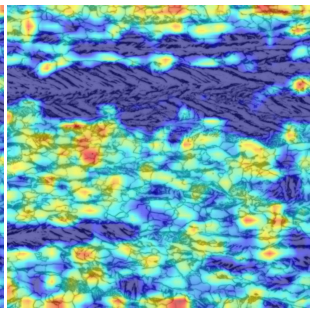

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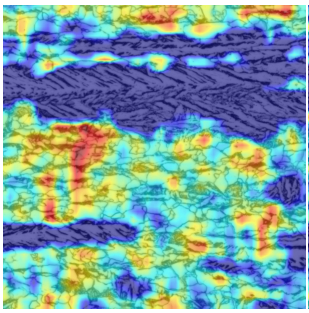

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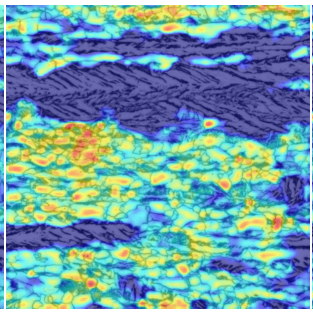
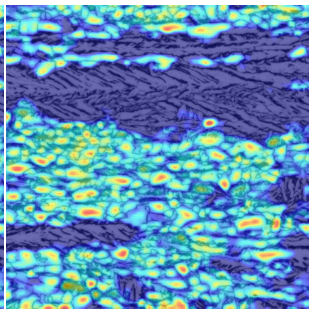


(6.14) up1.convr1



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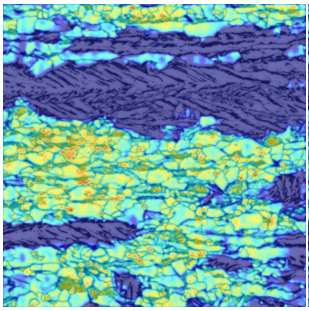
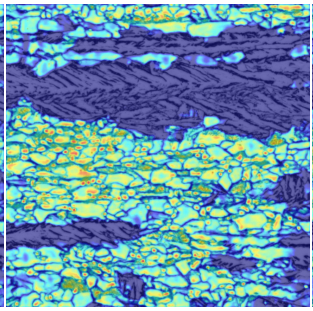
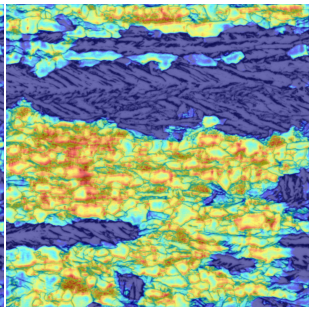


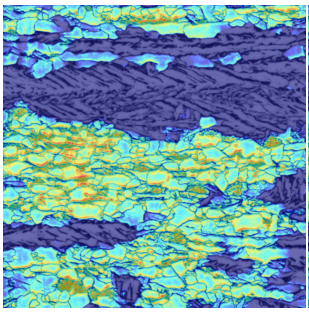
(6.16) up2.convr1



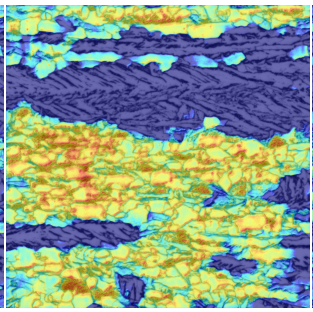
(6.17) up2.convr2



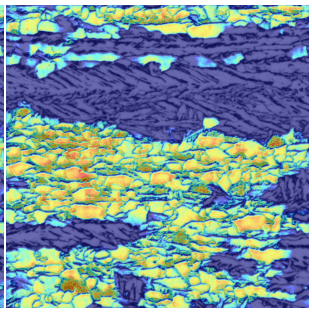
(6.18) up3.convr1



(6.19) up3.convr2



(6.20) up4.convr1



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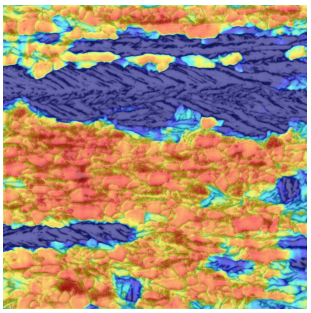
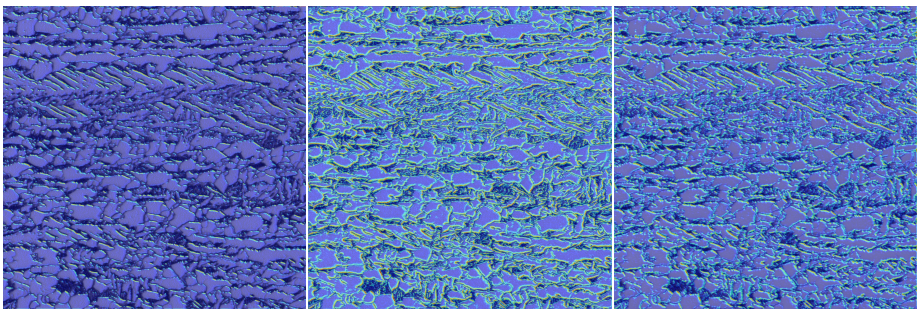
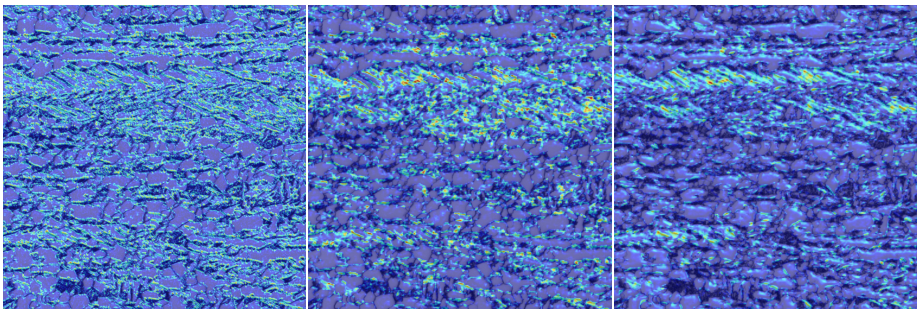


(6.22) output.seg.mask

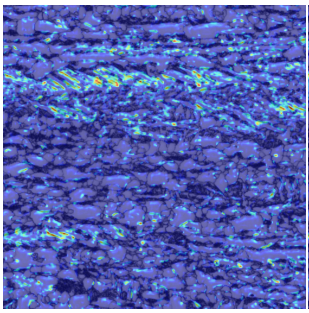
Supplementary Figure 7: Grad-CAM maps indicating image regions that dictated the decision of the VGG U-Net network with respect to the foreground class. The individual panel captions refer to the specific network layer for which the activation map is computed (see Supplemental Figure 1 and 2).



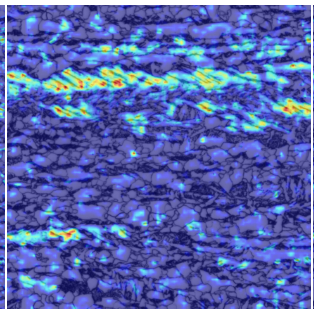
(7.1) down1.convr1 (7.2) down1.convr2 (7.3) down2.convr1



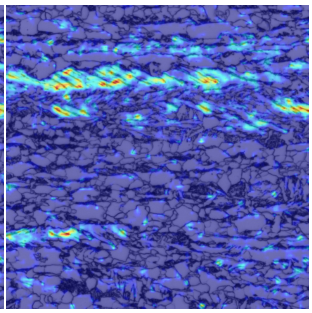
(7.4) down2.convr2 (7.5) down3.convr1 (7.6) down3.convr2



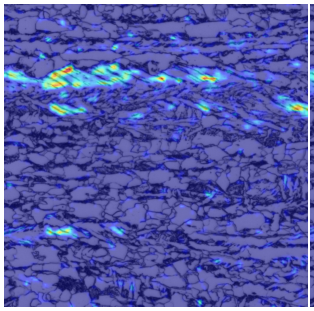
(7.7) down3.convr3



(7.8) down4.convr1



(7.9) down4.convr2



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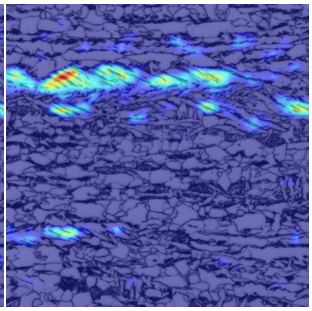

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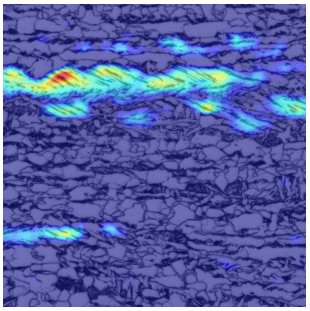

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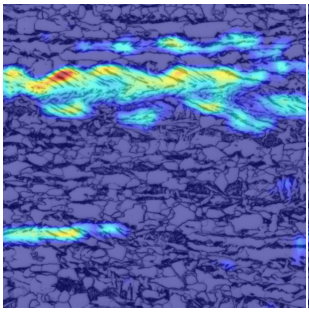

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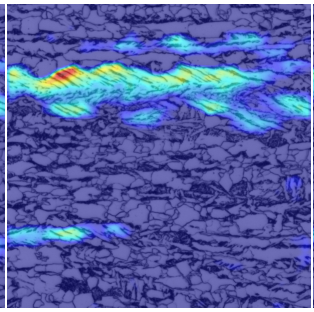
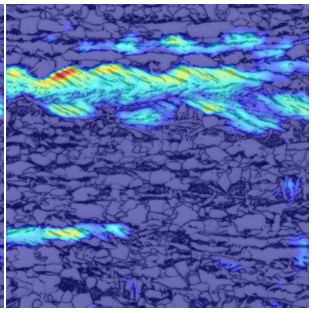
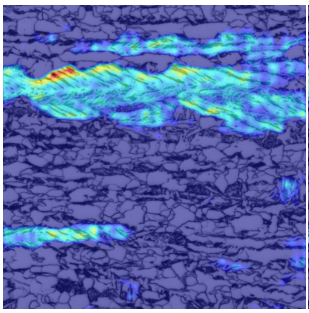


(7.14) up1.convr1



(7.15) up1.convr2



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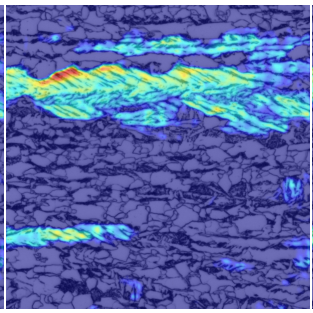

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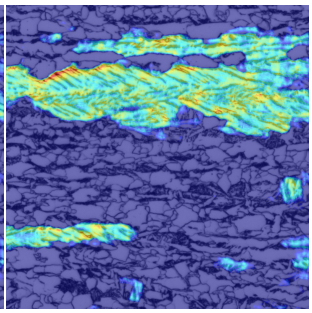

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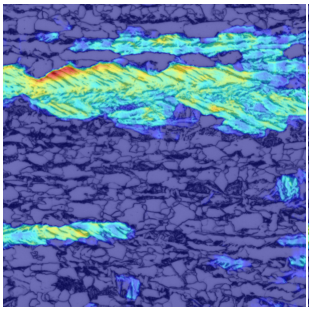

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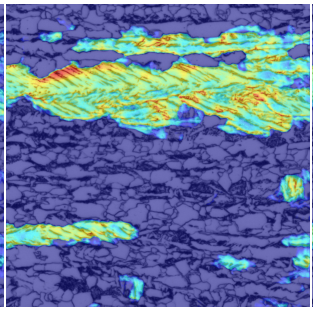
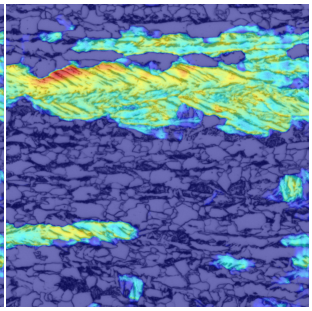
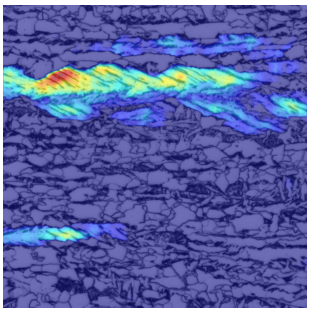


(7.20) up4.convr1



(7.21) up4.convr2



(7.22) output.seg.mask