Supplementary Materials: Appendix

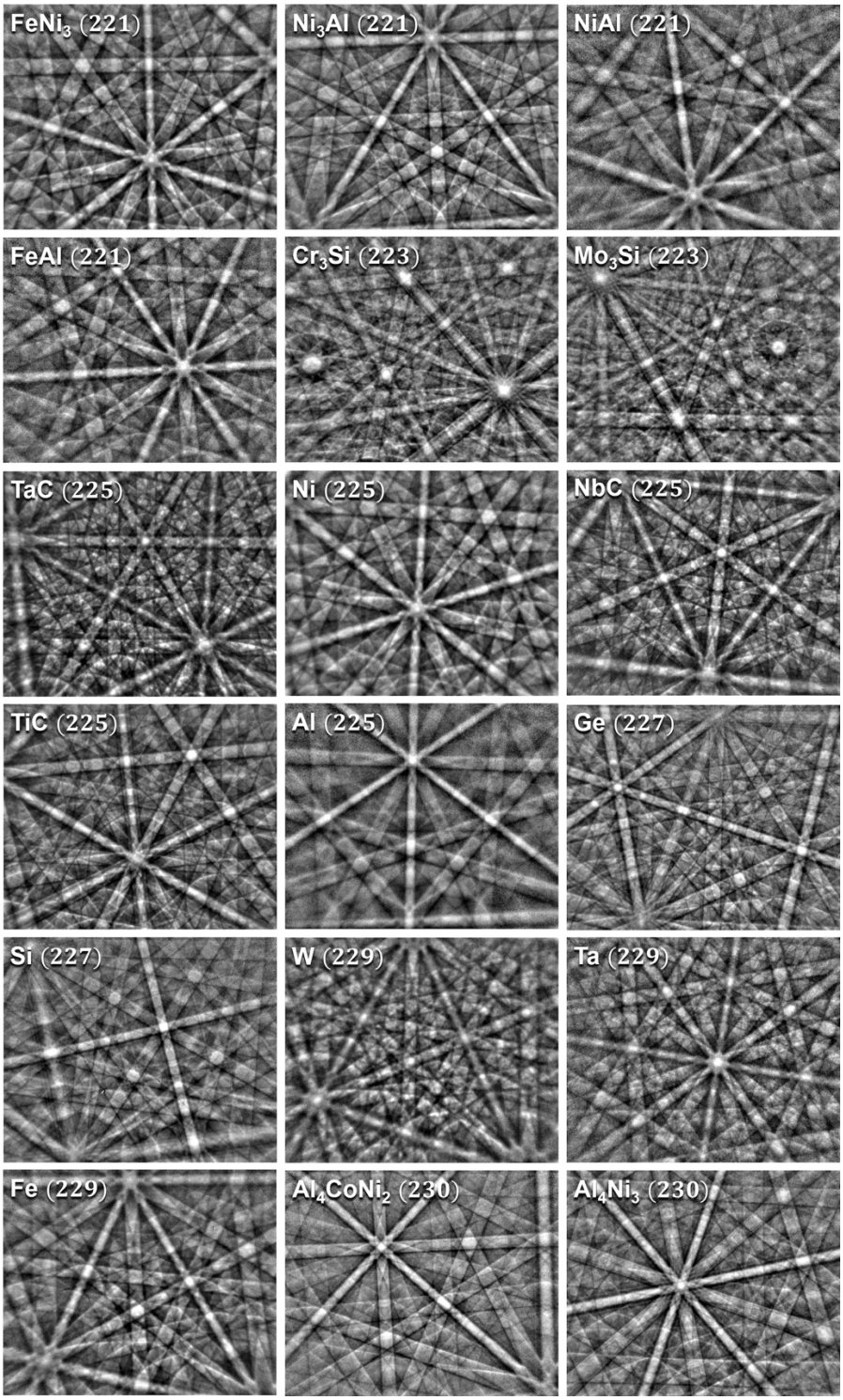

Fig. A1: Representative diffraction patterns from each material studied. The space group and material are denoted in the upper left corner of each diffraction pattern.

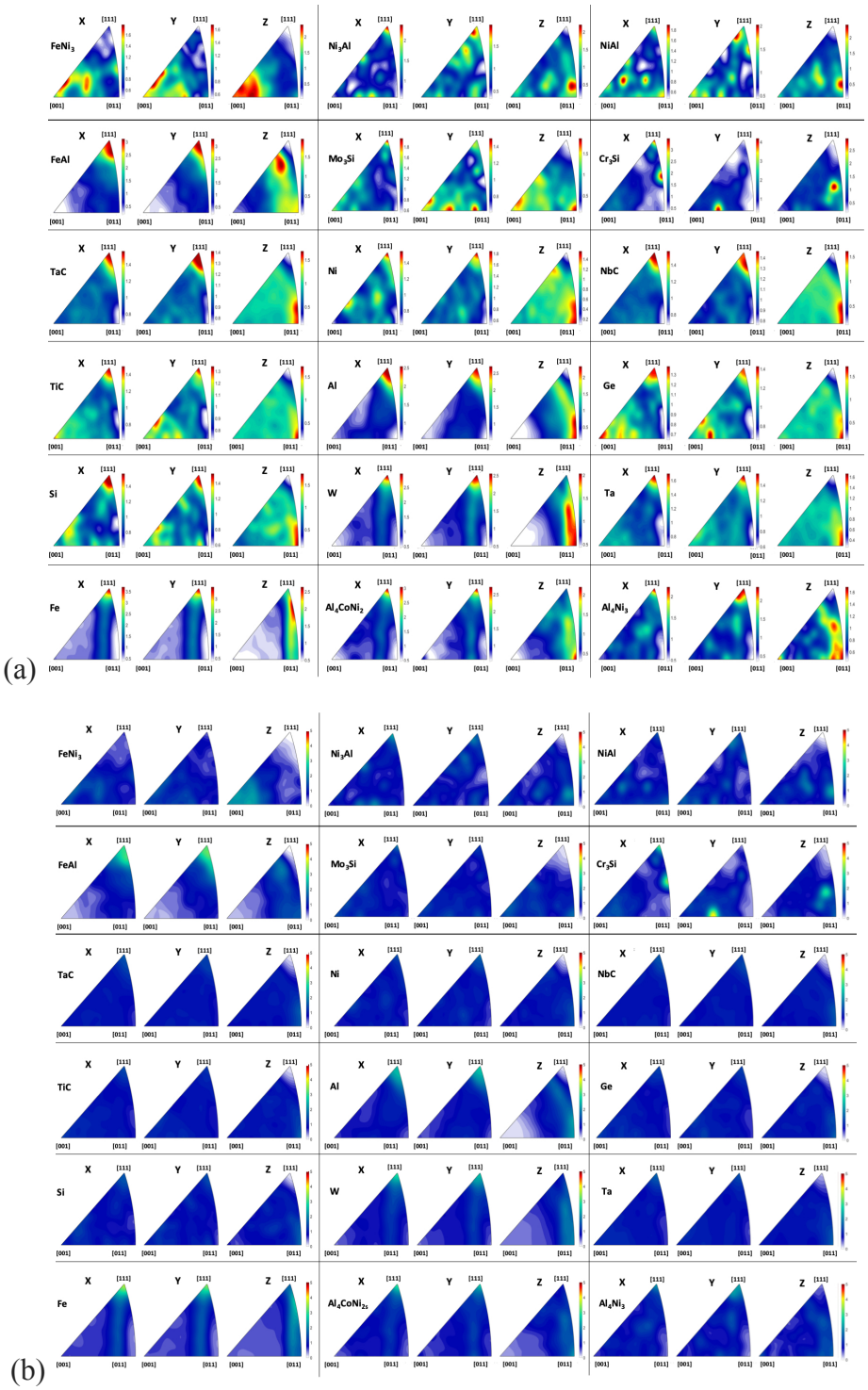

Fig. A2: Inverse pole figures of the entire dataset. Orientation analysis shows the materials are of very low texture, typically in the range of 2-3 multiples of uniform density (M.U.D.). Note that all of the data is below 5 M.U.D, the standard onset for medium texture. The data is first plotted (a) with the scale bars automatically determined by MTEX to show the data distribution. The second set of plots (b) uses the fixed scale of 0 to 5 M.U.D. to demonstrate that the data does not approach medium texture levels.

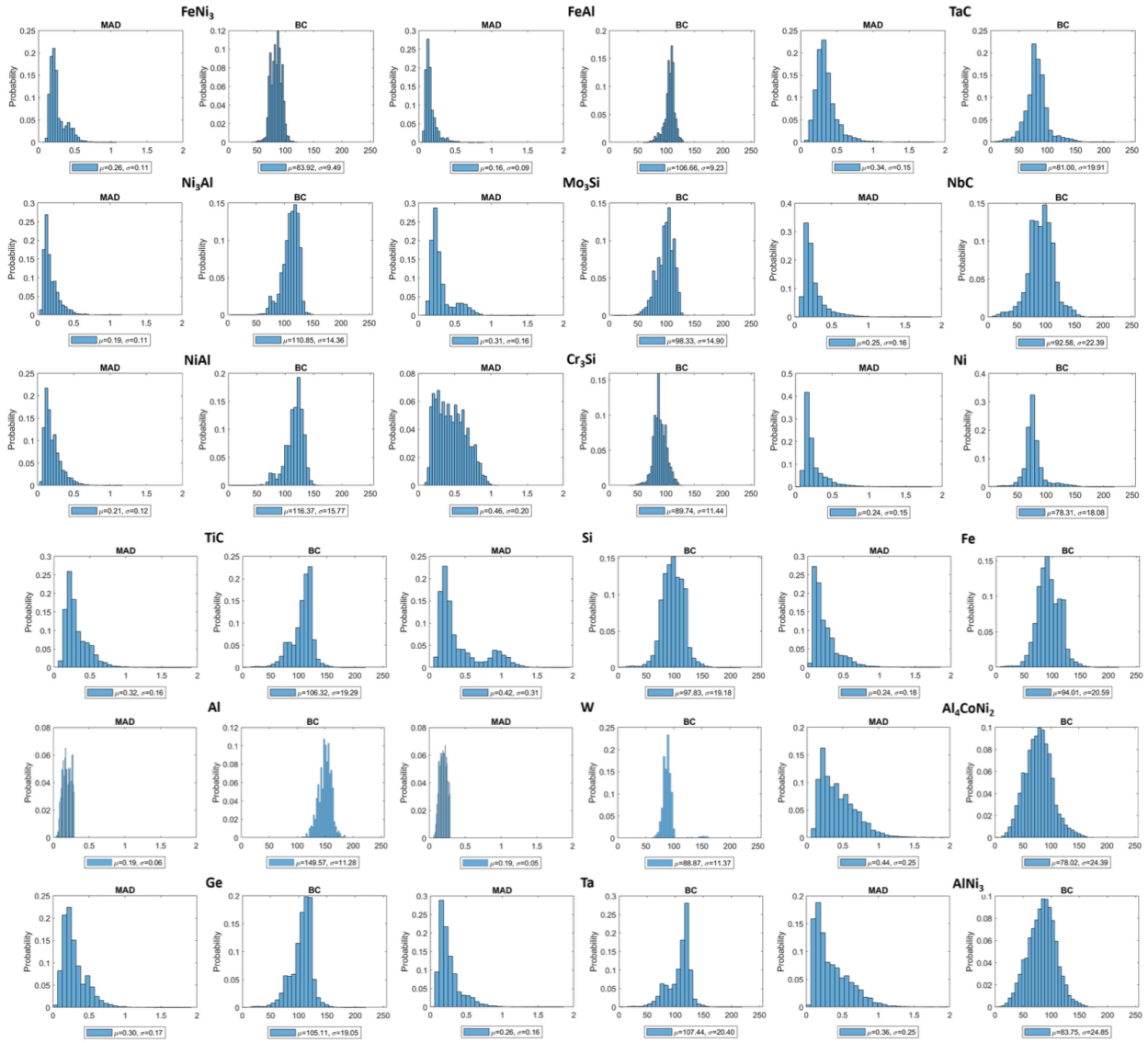

Fig. A3: Probability plots of mean angular deviation and band contrast for the entire dataset. The pattern quality distribution of each material is assessed using mean angular deviation (MAD) and band contrast (BC) as descriptors. Each plot is also annotated with the mean (μ) and standard deviation (σ).

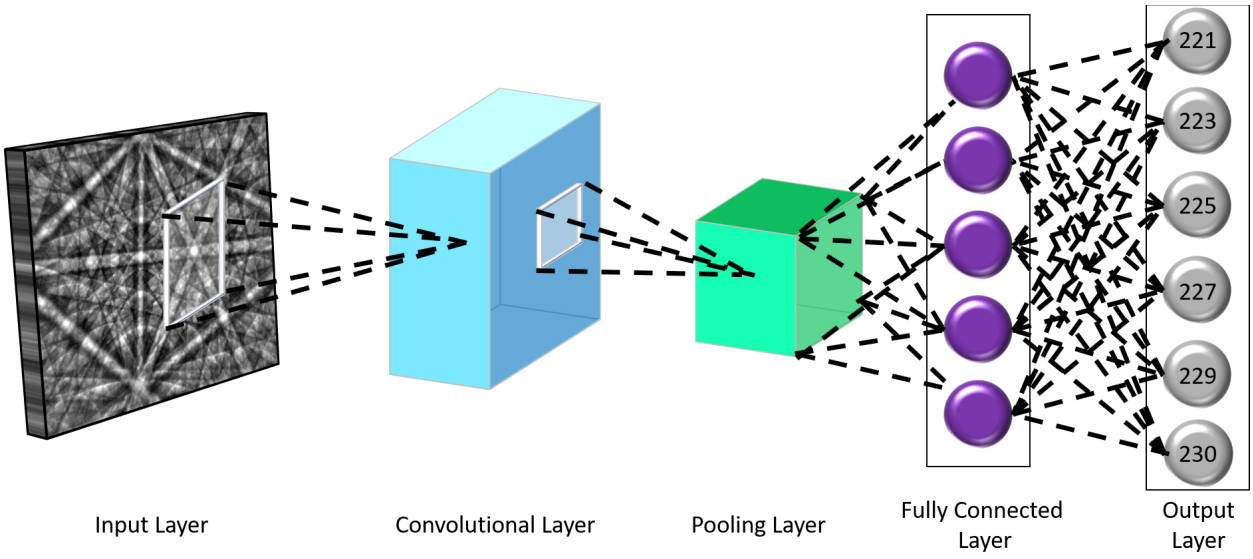

Fig. A4: Schematic of the neural network. In convolutional layers, a learnable filter is convolved across the image and the scalar product between the filter and the input at every position is computed to form a feature map. Pooling layers are placed after convolutional layers to down sample the feature maps and produce coarse grain representations and spatial information about the features in the data. A traditional dense neural network is placed as the last layer, where the probability that the input diffraction pattern belongs to each space group is computed.

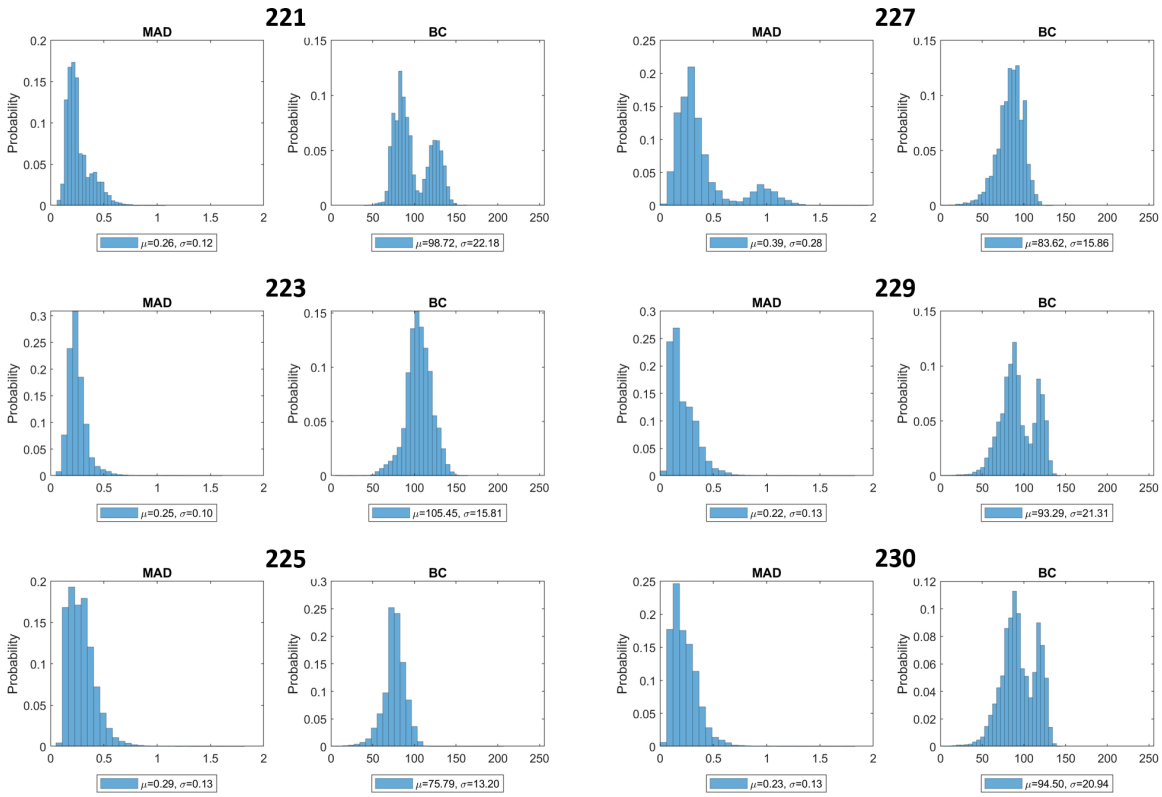

Fig. A5: Inverse pole figures for each space group training set in the associated model. The range of possible orientations are well represented for each class. Note that the scale bars are all below 5 M.U.D.

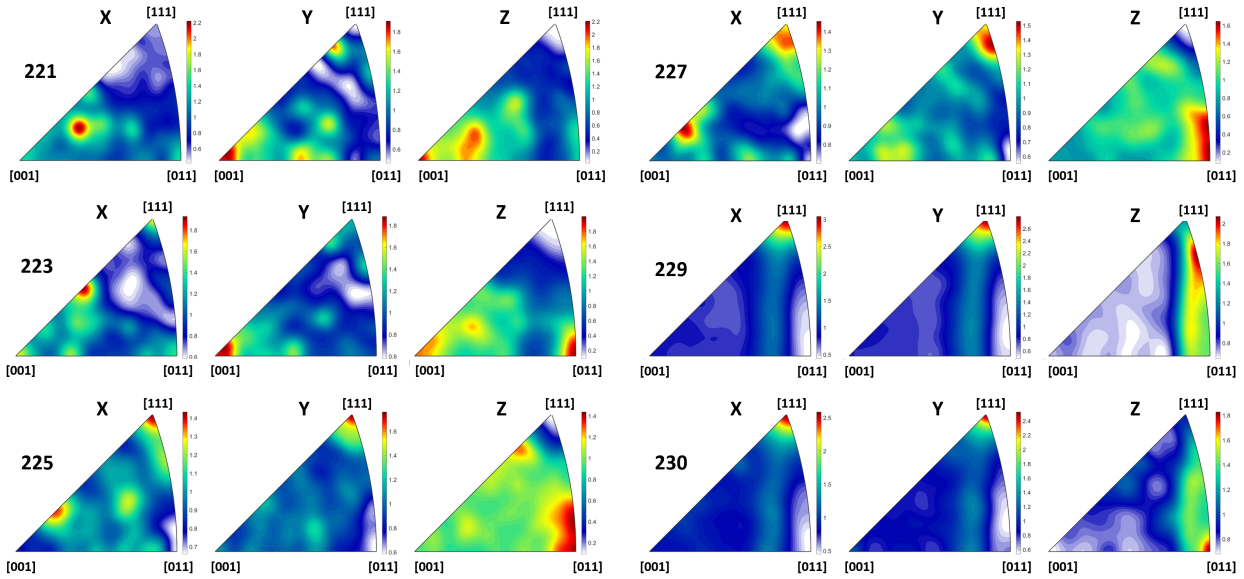

Fig. A6: Histograms of mean angular deviation and band contrast in the training set for the associated model. The pattern quality distribution of each material is assessed using mean angular deviation (MAD) and band contrast (BC) as descriptors. Each plot is also annotated with the mean (μ) and standard deviation (σ).

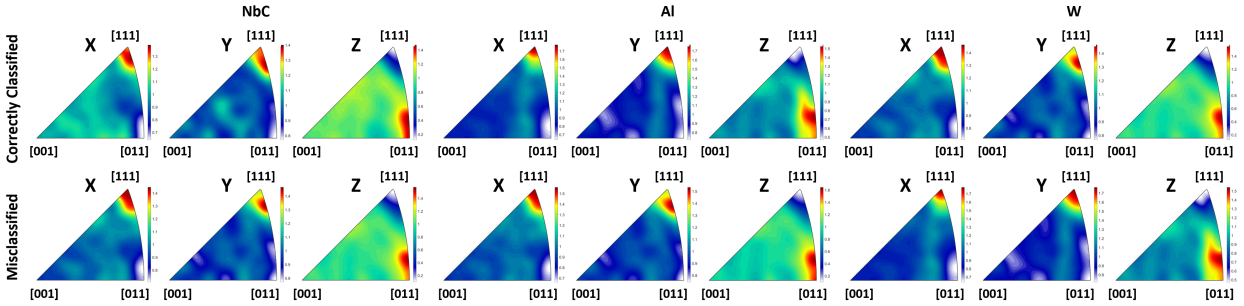

Fig. A7: Inverse pole figures for patterns based on correct or incorrect classification. The distribution of orientations that were correctly classified and misclassified are very similar, suggesting texture is not having a profound effect. Note that the scale bars are all below 5 M.U.D.

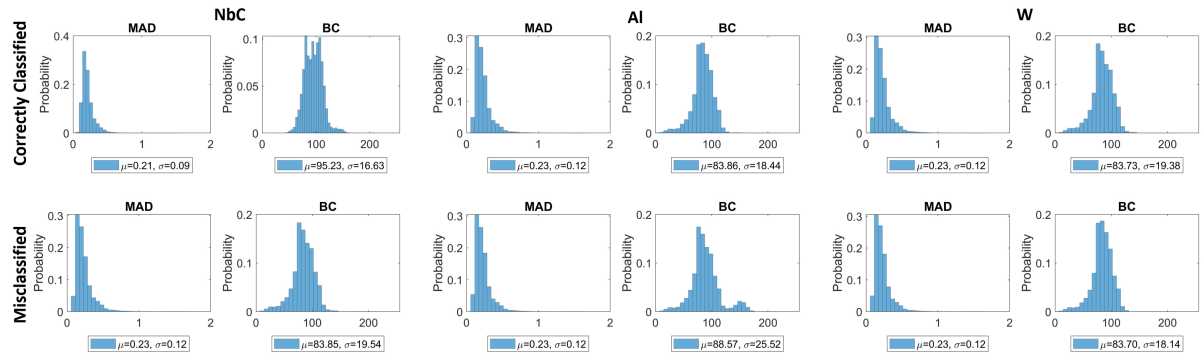

Fig. A8: Histograms of mean angular deviation and band contrast separated by correct or incorrect classification. The pattern quality distribution of each material is assessed using mean angular deviation (MAD) and band contrast (BC) as descriptors. Each plot is also annotated with the mean (μ) and standard deviation (σ).

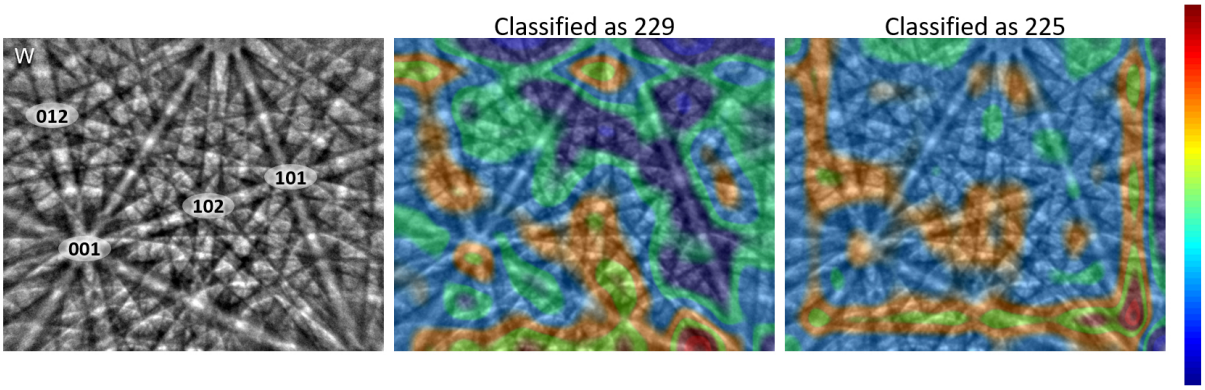

Fig. A9. Feature comparison for correct and incorrect classifications. The activations for the 229 class are studied when the pattern is correctly identified (middle) and misclassified to 255 (right). Similar information is identified; however, the zone axis activations are weaker for the misclassified pattern.

Table A1. Material acquisition and processing. The method of fabrication is listed for each material studied. SPS denotes spark plasma sintering from a commercial powder. The homogenization heat treatments were performed for one week in an inert atmosphere.

Space Group	Material	Formula Weighted Atomic Number	Method of Fabrication			
221			**Wrought**	**Arc Melt**	**SPS**	**Heat Treatment**
	FeNi3	27.5		X		X
	Ni3Al	24.25		X		X
	NiAl	20.5		X		X
	FeAl	19.5		X		X
223						
	Mo3Si	35		X		X
	Cr3Si	21.5		X		X
225						
	TaC	39.5			X	
	Ni	28	X			
	NbC	23.5			X	
	TiC	14			X	
	Al	13	X			
227						
	Ge	32		X		
	Si	14		X		
229						
	W	74			X	
	Ta	73			X	
	Fe	26		X		
230						
	Al4CoNi2	19.4		X		X
	Al4Ni3	19.4		X		X

Table A2. Number of diffraction patterns classified to each space group. Space group 221; trained on $FeNi_3$. Space group 223; trained on Mo_3Si. Space group 225; trained on TaC. Space group 227; trained on Ge. Space group 229; trained on Ta. Space group 230; trained on Al_4CoNi_2.

Space Group	Material	Formula Weighted Atomic Number	Number of Patterns Classified to Each Space Group						Accuracy	Precision	Recall
221			**221**	223	225	227	229	230			
	FeNi3	27.5	**9,987**	0	0	0	31	1	99.7%	0.24	1.00
	Ni3Al	24.25	**9,085**	0	6	0	42	400	95.3%	0.22	0.95
	NiAl	20.5	**79**	1	71	1	52	4,336	1.7%	0	0.02
	FeAl	19.5	**248**	0	0	1	1,538	76	13.3%	0.01	0.13
223			221	**223**	225	227	229	230			
	Cr3Si	21.5	11	**12,219**	0	0	357	1	97.1%	0.61	0.97
	Mo3Si	35	27	**10,498**	11	0	118	6	98.5%	0.57	0.99
225			221	223	**225**	227	229	230			
	TaC	39.5	527	97	**14,143**	10	462	44	92.5%	0.97	0.93
	Ni	28	11,170	8	**29**	1	424	82	0.2%	0.06	0.02
	NbC	23.5	776	698	**832**	15	16,222	57	4.5%	0.66	0.05
	TiC	14	12,381	398	**0**	0	2,778	35	0.0%	0	0
	Al	13	0	0	**0**	0	3	1,085	0.0%	0	0
227			221	223	225	**227**	229	230			
	Ge	32	1	14	0	**2,212**	12	1	98.8%	0.98	0.99
	Si	14	1,330	6,455	0	**1**	315	637	0.0%	0.03	0
229			221	223	225	227	**229**	230			
	W	74	150	140	281	0	**492**	0	46.3%	0.02	0.46
	Ta	73	1	1	17	1	**8,771**	4	99.7%	0.28	1
	Fe	26	5,899	64	25	3	**1,835**	1,690	19.3%	0.08	0.19
230			221	223	225	227	229	**230**			
	Al4CoNi2	19.4	1	1	2	1	2	**1,822**	99.6%	0.18	1
	Al4Ni3	19.4	30	4	16	5	31	**1,706**	95.2%	0.17	0.95
Total Patterns	144,465		221	223	225	227	229	230	Average		
# Correct	73,959	Precision	0.38	0.74	0.97	0.98	0.33	0.29	0.73		
Accuracy (%)	51.20	Recall	0.75	0.98	0.24	0.2	0.57	0.97	0.51		

Table A3. Number of diffraction patterns classified to each space group. Space group 221; trained on $FeNi_3$. Space group 223; trained on Mo_3Si. Space group 225; trained on Al. Space group 227; trained on Ge. Space group 229; trained on Ta. Space group 230; trained on Al_4CoNi_2.

Space Group	Material	Formula Weighted Atomic Number	Number of Patterns Classified to Each Space Group						Accuracy	Precision	Recall
221			**221**	223	225	227	229	230			
	FeNi3	27.5	**10,008**	3	2	0	6	0	99.9%	0.33	1.00
	Ni3Al	24.25	**8,733**	9	613	45	34	99	91.6%	0.3	0.92
	NiAl	20.5	**2**	0	4,345	2	30	161	0.0%	0	0
	FeAl	19.5	**67**	34	334	4	1,389	35	3.6%	0	0.04
223			221	**223**	225	227	229	230			
	Mo3Si	35	0	**10,614**	15	0	22	9	99.6%	0.28	1
	Cr3Si	21.5	0	**12,328**	1	0	259	0	97.9%	0.32	0.98
225			221	223	**225**	227	229	230			
	TaC	39.5	593	7,430	**115**	31	6,802	312	0.8%	0.01	0.01
	Ni	28	11,377	5	**196**	0	93	43	1.7%	0.02	0.02
	NbC	23.5	497	4,293	**179**	76	12,877	678	1.0%	0.02	0.01
	TiC	14	3,356	8,532	**3,537**	10	157	0	22.7%	0.25	0.23
	Al	13	0	0	**1,086**	1	0	1	99.8%	0.09	1
227			221	223	225	**227**	229	230			
	Ge	32	0	0	3	**2,236**	0	1	99.8%	0.86	1
	Si	14	402	4,829	2,566	**896**	15	30	10.3%	0.71	0.1
229			221	223	225	227	**229**	230			
	W	74	505	369	0	0	**189**	0	17.8%	0.01	0.18
	Ta	73	1	6	19	1	**8,766**	2	99.7%	0.29	1
	Fe	26	3,591	1,130	2,308	38	**2,236**	213	23.5%	0.09	0.23
230			221	223	225	227	229	**230**			
	Al4CoNi2	19.4	0	0	0	1	1	**1,827**	99.9%	0.54	1
	Al4Ni3	19.4	6	0	229	164	14	**1,379**	77.0%	0.47	0.77
Total Patterns	144,465		221	223	225	227	229	230	Average		
# Correct	64,394	Precision	0.48	0.46	0.33	0.89	0.34	0.67	0.43		
Accuracy (%)	44.57	Recall	0.72	0.99	0.08	0.29	0.58	0.89	0.44		

Table A4. Number of diffraction patterns classified to each space group. Space group 221; trained on $FeNi_3$. Space group 223; trained on Mo_3Si. Space group 225; trained on TaC. Space group 227; trained on Si. Space group 229; trained on Ta. Space group 230; trained on Al_4CoNi_2.

Space Group	Material	Formula Weighted Atomic Number	Number of Patterns Classified to Each Space Group						Accuracy	Precision	Recall
221			**221**	223	225	227	229	230			
	FeNi3	27.5	**10,000**	4	1	10	4	0	99.8%	0.22	1.00
	Ni3Al	24.25	**9,357**	25	4	41	30	76	98.2%	0.21	0.98
	NiAl	20.5	**990**	0	66	65	174	3,245	21.8%	0.03	0.22
	FeAl	19.5	**909**	55	0	15	776	108	48.8%	0.02	0.49
223			221	**223**	225	227	229	230			
	Mo3Si	35	0	**10,629**	7	13	9	2	99.7%	0.75	1
	Cr3Si	21.5	0	**12,454**	7	121	6	0	98.9%	0.78	0.99
225			221	223	**225**	227	229	230			
	TaC	39.5	192	26	**14,752**	115	176	22	96.5%	0.93	0.97
	Ni	28	11,477	2	**28**	103	84	20	0.2%	0.03	0
	NbC	23.5	3,014	470	**7,353**	255	7,478	30	39.5%	0.88	0.4
	TiC	14	12,916	53	**53**	2,554	16	0	0.3%	0.05	0
	Al	13	479	0	**0**	17	9	583	0.0%	0	0
227			221	223	225	**227**	229	230			
	Ge	32	1	2,076	0	**83**	72	8	3.7%	0.02	0.04
	Si	14	2	9	0	**8,726**	0	1	99.9%	0.69	1
229			221	223	225	227	**229**	230			
	W	74	119	2	901	7	**34**	0	3.2%	0	0.03
	Ta	73	2	3	10	3	**8,775**	2	99.8%	0.5	1
	Fe	26	7,259	688	20	655	**689**	205	7.2%	0.07	0.07
230			221	223	225	227	229	**230**			
	Al4CoNi2	19.4	0	0	2	0	5	**1,822**	99.6%	0.3	1
	Al4Ni3	19.4	65	79	16	13	24	**1,595**	89.0%	0.27	0.89
Total Patterns	144,465		221	223	225	227	229	230	Average		
# Correct	88,249	Precision	0.37	0.87	0.96	0.69	0.52	0.44	0.75		
Accuracy (%)	61.09	Recall	0.82	0.99	0.36	0.8	0.49	0.94	0.61		

Table A5. Number of diffraction patterns classified to each space group. Space group 221; trained on $FeNi_3$. Space group 223; trained on Mo_3Si. Space group 225; trained on TaC. Space group 227; trained on Ge. Space group 229; trained on Fe. Space group 230; trained on Al_4CoNi_2.

Space Group	Material	Formula Weighted Atomic Number	Number of Patterns Classified to Each Space Group						Accuracy	Precision	Recall
221			**221**	223	225	227	229	230			
	FeNi3	27.5	**10,004**	3	0	0	12	0	99.9%	0.38	1.00
	Ni3Al	24.25	**9,129**	11	1	3	902	87	95.8%	0.35	0.96
	NiAl	20.5	**13**	9	68	67	1,901	2,482	0.3%	0	0
	FeAl	19.5	**3**	19	0	26	1,811	4	0.2%	0	0
223			221	**223**	225	227	229	230			
	Mo3Si	35	2	**10,630**	12	4	10	2	99.7%	0.46	1
	Cr3Si	21.5	10	**12,575**	0	3	0	0	99.9%	0.5	1
225			221	223	**225**	227	229	230			
	TaC	39.5	112	116	**14,889**	34	118	14	97.4%	0.89	0.97
	Ni	28	11,016	11	**46**	10	609	22	0.4%	0.02	0
	NbC	23.5	126	1,123	**14,173**	167	2,965	46	76.2%	0.88	0.76
	TiC	14	4,634	1,922	**11**	68	8,957	0	0.1%	0.01	0
	Al	13	9	1	**0**	14	67	997	0.0%	0	0
227			221	223	225	**227**	229	230			
	Ge	32	0	0	0	**2,237**	1	2	99.9%	0.8	1
	Si	14	504	6,358	1	**242**	1,282	351	2.8%	0.3	0.03
229			221	223	225	227	**229**	230			
	W	74	26	44	963	0	**30**	0	2.8%	0	0.03
	Ta	73	52	2,934	788	106	**4,913**	2	55.9%	0.21	0.56
	Fe	26	113	31	32	2	**9,329**	9	98.0%	0.34	0.98
230			221	223	225	227	229	**230**			
	Al4CoNi2	19.4	0	0	5	2	0	**1,822**	99.6%	0.31	1
	Al4Ni3	19.4	9	10	14	52	90	**1,617**	90.2%	0.29	0.9
Total Patterns	144,465		221	223	225	227	229	230	Average		
# Correct	91,663	Precision	0.54	0.65	0.94	0.82	0.44	0.46	0.73		
Accuracy (%)	63.45	Recall	0.74	1	0.47	0.23	0.74	0.95	0.63		

Table A6. Number of diffraction patterns classified to each space group. Space group 221; trained on $FeNi_3$ and NiAl. Space group 223; trained on Mo_3Si. Space group 225; trained on TaC and Ni. Space group 227; trained on Ge and Si. Space group 229; trained on Ta and Fe. Space group 230; trained on Al_4CoNi_2.

Space Group	Material	Formula Weighted Atomic Number	Number of Patterns Classified to Each Space Group						Accuracy	Precision	Recall
221			**221**	223	225	227	229	230			
	FeNi3	27.5	**8,124**	0	1,881	0	13	1	81.1%	0.32	0.81
	Ni3Al	24.25	**8,524**	0	979	0	28	2	89.4%	0.33	0.89
	NiAl	20.5	**4,537**	0	2	0	0	1	99.9%	0.21	1
	FeAl	19.5	**647**	0	143	0	1,073	0	34.7%	0.04	0.35
223			221	**223**	225	227	229	230			
	Mo3Si	35	100	**10,373**	21	2	161	3	97.3%	0.95	0.97
	Cr3Si	21.5	249	**11,403**	280	2	654	0	90.6%	0.96	0.93
225			221	223	**225**	227	229	230			
	TaC	39.5	577	90	**13,967**	77	562	10	91.4%	0.72	0.91
	Ni	28	362	1	**11,334**	0	8	9	96.8%	0.68	0.97
	NbC	23.5	1,462	261	**13,429**	122	3,290	36	72.2%	0.71	0.72
	TiC	14	9,899	8	**5,454**	0	231	0	35.0%	0.5	0.35
	Al	13	1,047	0	**33**	0	0	8	3.0%	0.01	0.03
227			221	223	225	**227**	229	230			
	Ge	32	141	34	0	**1,936**	127	2	86.4%	0.9	0.86
	Si	14	1,485	99	555	**6,387**	205	7	73.1%	0.97	0.73
229			221	223	225	227	**229**	230			
	W	74	9	1	1,012	0	**41**	0	3.9%	0.01	0.04
	Ta	73	139	0	40	2	**8,613**	1	97.9%	0.57	0.98
	Fe	26	884	0	462	0	**8,170**	0	85.9%	0.56	0.86
230			221	223	225	227	229	**230**			
	Al4CoNi2	19.4	16	0	0	0	1	**1,812**	99.1%	0.96	0.99
	Al4Ni3	19.4	591	0	0	2	38	**1,161**	64.8%	0.94	0.65
Total Patterns	144,465		221	223	225	227	229	230	Average		
# Correct	115,945	Precision	0.56	0.98	0.89	0.98	0.72	0.97	0.83		
Accuracy (%)	80.26	Recall	0.84	0.94	0.71	0.76	0.87	0.82	0.80		

Table A7. Number of diffraction patterns classified to each space group. The model was trained using a small subset of patterns from each of the available materials.

Space Group	Material	Formula Weighted Atomic Number	Number of Patterns Classified to Each Space Group						Accuracy	Precision	Recall
221			**221**	223	225	227	229	230			
	FeNi3	27.5	**9,370**	2	551	5	88	3	93.5%	0.65	0.94
	Ni3Al	24.25	**9,015**	1	378	22	77	40	94.6%	0.64	0.95
	NiAl	20.5	**4,381**	0	41	16	11	91	96.5%	0.46	0.96
	FeAl	19.5	**1,725**	0	6	0	131	1	92.6%	0.25	0.93
223			221	**223**	225	227	229	230			
	Mo3Si	35	14	**10,572**	1	76	33	9	98.8%	0.98	0.99
	Cr3Si	21.5	6	**12,544**	10	21	7	0	99.7%	0.98	1
225			221	223	**225**	227	229	230			
	TaC	39.5	115	132	**13,601**	695	719	21	89.0%	0.93	0.89
	Ni	28	3,160	1	**8,107**	32	381	33	69.2%	0.89	0.69
	NbC	23.5	272	19	**16,404**	1,304	553	48	88.2%	0.94	0.88
	TiC	14	166	34	**15,230**	52	110	0	97.7%	0.94	0.98
	Al	13	64	0	**1,015**	0	1	8	93.3%	0.5	0.93
227			221	223	225	**227**	229	230			
	Ge	32	5	1	0	**2,222**	6	6	99.2%	0.49	0.99
	Si	14	4	4	2	**8,720**	6	2	99.8%	0.79	1
229			221	223	225	227	**229**	230			
	W	74	0	0	3	0	**1,060**	0	99.7%	0.33	1
	Ta	73	105	0	4	24	**8,657**	5	98.4%	0.8	0.98
	Fe	26	1,148	16	37	21	**8,246**	48	86.7%	0.79	0.87
230			221	223	225	227	229	**230**			
	Al4CoNi2	19.4	3	0	0	7	1	**1,818**	99.4%	0.85	0.99
	Al4Ni3	19.4	30	0	0	23	9	**1,730**	96.5%	0.85	0.97
Total Patterns	144,465		221	223	225	227	229	230	Average		
# Correct	134,417	Precision	0.83	0.99	0.98	0.83	0.89	0.92	0.93		
Accuracy (%)	93.04	Recall	0.94	0.99	0.87	1	0.93	0.98	0.92		