Supporting Information for "FORCINN: First-order reversal curve inversion of magnetite using neural networks"

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Introduction This supplementary information contains the model description (Text S1), structure diagrams (Figures S1 and S2), and detailed parameter tables (Tables S1-S3) of the convolutional neural network (CNN) and residual neural network (ResNet) models used in this study, as well as prediction results of models trained with different noise levels on five experimental FORC data (Tables S4-S8).

Text S1: Hidden layers of CNN and ResNet

The hidden layers of the CNN model consist of five sets of 3×3 padded convolutional (two 64-channels, two 128-channels, and one 256-channel) and 2×2 max-pooling layers, a flattening layer, and a 256-dimensional fully connected layer, all with rectified linear unit (ReLU) activation functions (Figure S1, Table S1)(LeCun et al., 2015).

The hidden layers of the ResNet model consist of a convolutional block, five ResNet blocks (two 64-channels, two 128-channels, and one 256-channel), and a global average pooling layer (Figure S2, Table S2) (He et al., 2016). The convolutional block starts with a 3×3 padded convolutional layer (64-channel), followed by a batch normalization layer, a ReLU activation function, and a 2×2 max-pooling layer (Figure S2, Table S2). Each ResNet block contains two 3×3 padded convolutional layers and a shortcut connection with a 1×1 padded convolutional layer, each followed by a batch normalization layer (Figure S2, Table S3). ReLU activation function is used for the first convolutional layer and the shortcut connection layer. Each ResNet block is followed by a 30% dropout layer.

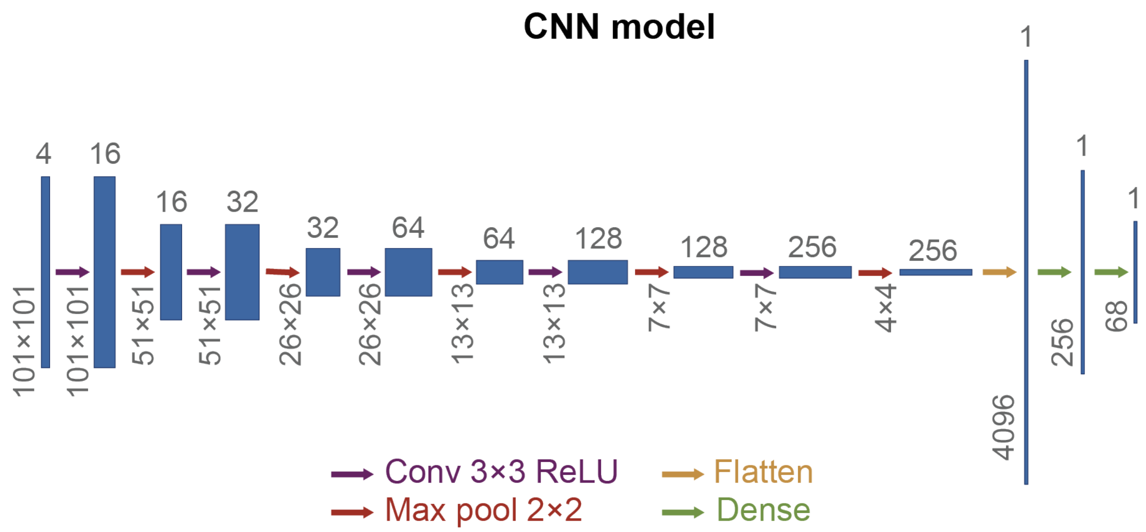

Figure S1. Model structure of the CNN model.

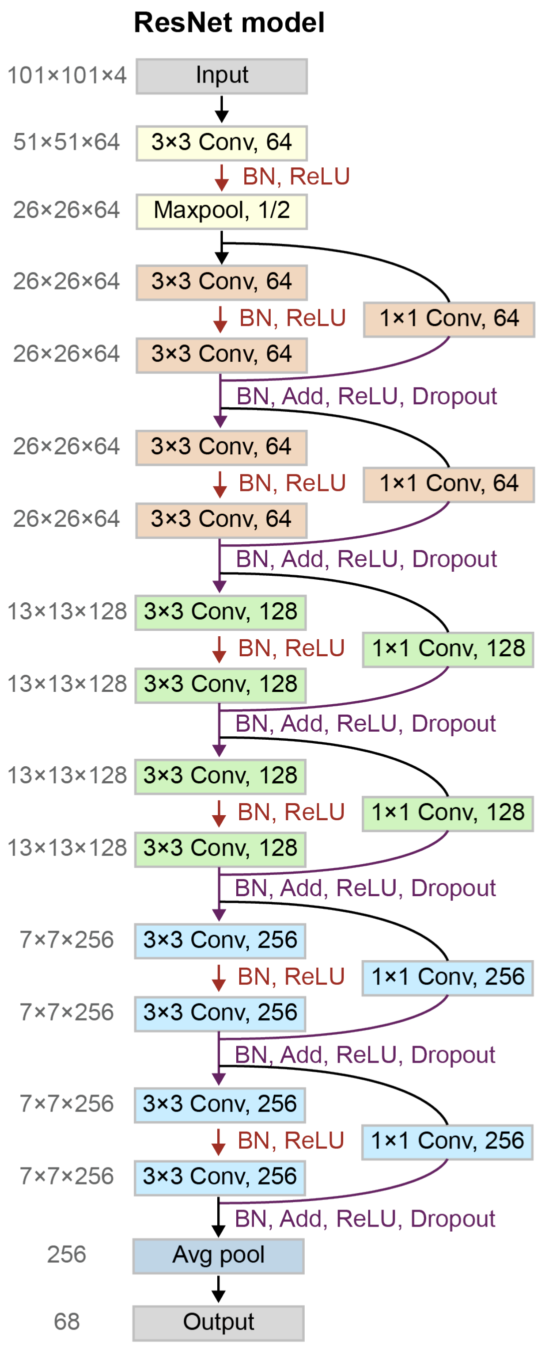

Figure S2. Model structure of the ResNet model.

Table S1. Model summary and parameters of the CNN.

Layer type	Output shape	Param #
Input	(101, 101, 4)	-
Conv2D	(101, 101, 64)	2368
MaxPooling2D	(51, 51, 64)	0
Dropout	(51, 51, 64)	0
Conv2D	(51, 51, 64)	36928
MaxPooling2D	(26, 26, 64)	0
Dropout	(26, 26, 64)	0
Conv2D	(26, 26, 128)	73856
MaxPooling2D	(13, 13, 128)	0
Dropout	(13, 13, 128)	0
Conv2D	(13, 13, 128)	147584
MaxPooling2D	(7, 7, 128)	0
Dropout	(7, 7, 128)	0
Conv2D	(7, 7, 256)	36928
MaxPooling2D	(4, 4, 256)	0
Dropout	(4, 4, 256)	0
Flatten	(4096)	0
Dense	(256)	1048832
Dropout	(256)	0
Dense	(68)	17476

Table S2. Model summary and parameters of the ResNet. The details of the ResNet block can be found at Table S3.

Layer type	Output shape	Param #
Input	(101, 101, 4)	-
Conv2D	(51, 51, 64)	2368
BatchNormalization	(51, 51, 64)	256
ReLU	(51, 51, 64)	0
MaxPooling2D	(26, 26, 64)	0
ResNet Block	(26, 26, 64)	78784
ResNet Block	(26, 26, 64)	78784
ResNet Block	(13, 13, 128)	231026
ResNet Block	(13, 13, 128)	313216
ResNet Block	(7, 7, 256)	921344
ResNet Block	(7, 7, 256)	1249024
GlobeAveragePooling2D	(256)	0
Dense	(68)	17476

Table S3. Model summary and parameters of the ResNet block. X is the input size. C_1 is the number of input channels. C_2 is the number of convolution kernels in this block.

Layer	Output shape	Param #	Connected to
Conv2D_1	(X, X, C_2)	$(9C_1 + 1)C_2$	Input
BatchNormalization_1	(X, X, C_2)	$4C_2$	Conv2D_1
ReLU_1	(X, X, C_2)	0	BatchNormalization_1
Conv2D_2	(X, X, C_2)	$(9C_2 + 1)C_2$	ReLU_1
Conv2D_3	(X, X, C_2)	$(C_1 + 1)C_2$	Input
BatchNormalization_2	(X, X, C_2)	$4C_2$	Conv2D_2
BatchNormalization_3	(X, X, C_2)	$4C_2$	Conv2D_3
Add	(X, X, C_2)	0	[BatchNormalization_2, BatchNormalization_3]
ReLU_2	(X, X, C_2)	0	Add
Dropout	(X, X, C_2)	0	ReLU_2

Table S4. Prediction results of trained CNN and ResNet models at different noise levels for Hekla sample. The mean/median size of sample is 87.60/70.73 nm, and the mean/median aspect ratio is 1.24/1.21.

Model	Noise	Predicted size (nm)		Predicted aspect ratio	
		Mean/median	P-value	Mean/median	P-value
CNN	0	88.95/85	0.0011	1.45/1.45	0.0504
CNN	5%	88.22/85	0.0001	1.46/1.45	0.0048
CNN	10%	83.42/80	0.0011	1.46/1.45	0.1729
CNN	20%	92.75/90	0.0011	1.53/1.50	0.1729
ResNet	0	82.80/80	0.0000	1.53/1.50	0.0965
ResNet	5%	96.80/90	0.0153	1.81/1.80	0.0007
ResNet	10%	119.68/105	0.8745	1.57/1.50	0.0247
ResNet	20%	111.34/100	0.9794	1.53/1.50	0.0247

Table S5. Prediction results of trained CNN and ResNet models at different noise levels for Vesuvius sample. The mean/median size of sample is 174.35/135.90 nm, and the mean/median aspect ratio is 1.37/1.36.

Model	Noise	Predicted size (nm)		Predicted aspect ratio	
		Mean/median	P-value	Mean/median	P-value
CNN	0	100.83/95	0.0000	2.19/2.25	0.4535
CNN	5%	85.85/85	0.0000	1.39/1.40	0.0019
CNN	10%	86.88/85	0.0000	1.38/1.35	0.0048
CNN	20%	93.17/90	0.0000	1.35/1.35	0.0001
ResNet	0	103.77/85	0.0000	1.71/1.70	0.1729
ResNet	5%	92.66/85	0.0000	2.15/2.00	0.0048
ResNet	10%	130.58/90	0.0011	1.45/1.45	0.0000
ResNet	20%	146.57/120	0.3235	1.42/1.40	0.0048

Table S6. Prediction results of trained CNN and ResNet models at different noise levels for MD2361-125 sample. The mean/median size of sample is 67.95/65.17 nm, and the mean/median aspect ratio is 1.46/1.14.

Model	Noise	Predicted size (nm)		Predicted aspect ratio	
		Mean/median	P-value	Mean/median	P-value
CNN	0	98.25/95	0.0153	1.37/1.35	0.6543
CNN	5%	94.56/95	0.0153	1.45/1.45	0.6543
CNN	10%	94.35/95	0.0153	1.02/1.00	0.6543
CNN	20%	96.97/95	0.0153	1.25/1.30	0.6543
ResNet	0	92.37/90	0.0153	1.31/1.30	0.2899
ResNet	5%	95.41/95	0.0153	1.71/1.60	0.0247
ResNet	10%	97.23/95	0.0153	1.66/1.60	0.0965
ResNet	20%	90.81/90	0.0153	1.47/1.45	0.6543

Table S7. Prediction results of trained CNN and ResNet models at different noise levels for MD2361-315 sample. The mean/median size of sample is 71.88/69.28 nm, and the mean/median aspect ratio is 1.42/1.21.

Model	Noise	Predicted size (nm)		Predicted aspect ratio	
		Mean/median	P-value	Mean/median	P-value
CNN	0	111.30/110	0.0153	1.15/1.10	0.6543
CNN	5%	101.42/100	0.0153	1.93/1.85	0.2899
CNN	10%	102.06/100	0.0153	1.66/1.60	0.0247
CNN	20%	106.12/105	0.0153	1.91/1.80	0.1729
ResNet	0	108.40/105	0.0153	1.37/1.30	0.6543
ResNet	5%	100.13/100	0.0153	1.90/1.80	0.2899
ResNet	10%	101.31/100	0.0153	1.92/1.85	0.4535
ResNet	20%	93.10/95	0.0153	1.80/1.75	0.4535

Table S8. Prediction results of trained CNN and ResNet models at different noise levels for powders sample. The mean/median size of all grains in sample is 385.92/305.76 nm, and the mean/median aspect ratio is 1.36/1.22 The mean/median of <400 nm grains in sample is 223.30/216.20 nm, and the mean/median aspect ratio is 1.28/1.13.

Model	Noise	Predicted size (nm)		Predicted aspect ratio	
		Mean/median	P-value	Mean/median	P-value
CNN	0	221.65/195	0.0000	2.65/2.50	0.0113
CNN	5%	162.09/150	0.0000	2.24/2.25	0.0113
CNN	10%	143.19/140	0.0000	2.44/2.25	0.0113
CNN	20%	146.74/140	0.0000	2.72/2.50	0.0113
ResNet	0	200.46/240	0.0000	2.21/2.25	0.0113
ResNet	5%	163.67/150	0.0000	2.50/2.50	0.0113
ResNet	10%	159.77/150	0.0000	2.59/2.50	0.0113
ResNet	20%	159.77/155	0.0000	2.81/2.75	0.0113

References

He, K., Zhang, X., Ren, S., & Sun, J. (2016). Deep residual learning for image recognition. In *Proceedings of the ieee conference on computer vision and pattern recognition* (pp. 770–778).

LeCun, Y., Bengio, Y., & Hinton, G. (2015). Deep learning. *nature*, *521*(7553), 436–444.