

Supporting Information

Study of the Freeze Casting Process by Artificial Neural Networks

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Table S1. Fitting parameters corresponding to Figures 2 and 3. N is the number of samples in the group. r and R^2 are the coefficients of correlation and determination, respectively. For all r and R^2 in this table, $p < 0.0001$. MAE is mean absolute error; MAPE is mean absolute percentage error. KS D-value and p-value are obtained from Kolmogorov-Smirnov test.

group name	N	r	R^2	MAE	MAPE (%)	KS D-value	KS p-value
ALL	625	0.82	0.67	0.0725	15.78	0.40	2.70E-91
water	457	0.82	0.67	0.0719	14.69	0.41	1.91E-68
camphene	71	0.80	0.64	0.0832	18.49	0.40	1.25E-10
TBA	97	0.81	0.65	0.0674	18.96	0.43	3.72E-17
ceramic	532	0.77	0.59	0.0770	17.15	0.40	1.48E-76
metal	38	0.75	0.51	0.0757	14.54	0.45	2.01E-07
polymer	55	0.94	0.82	0.0267	3.37	0.45	7.18E-11

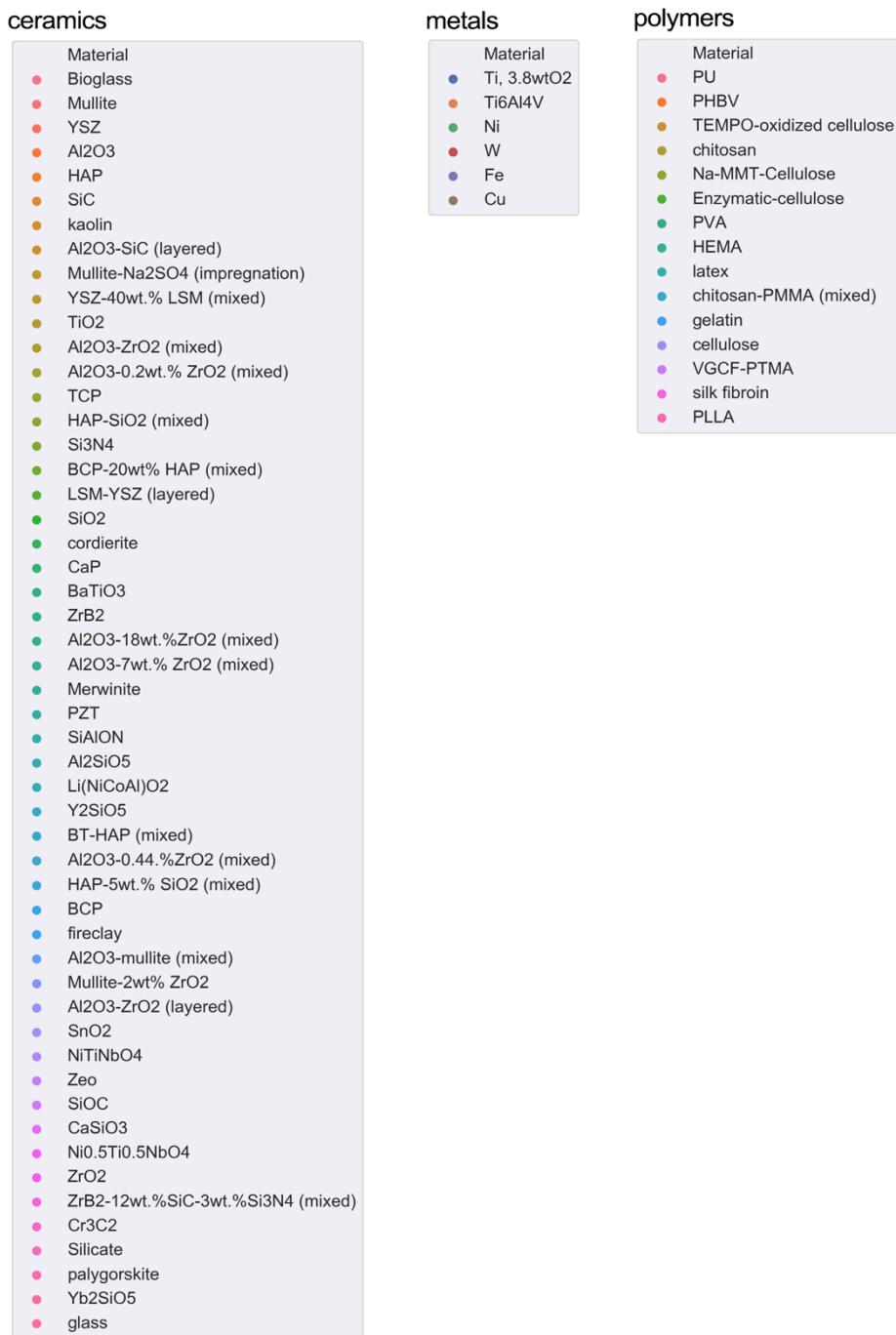


Figure S1. Legends of Figure 3c.

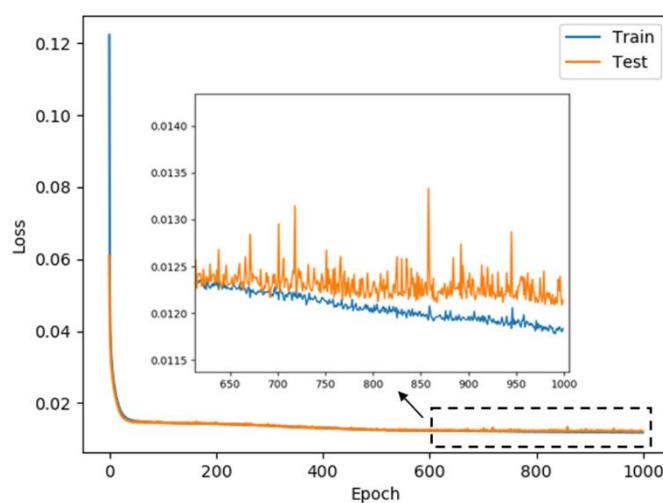


Figure S2. Loss decrease during ANN model training.

The screenshot shows a web-based application titled 'Predict Porosity'. The main heading says 'Now you get a predicted porosity by ANN'. Below this are four input fields: 'Material Group' (set to 'metal'), 'Solid Material' (set to 'Fe'), 'Solvent' (set to 'camphene'), and 'Volume Fraction of Solid' (set to '0.85'). At the bottom, there is a 'Predicted Porosity' section with a 'Calculate' button, a display field showing '0.25143096', and a 'Clear' button.

Figure S3. The interface of the ANN-prediction tool.

Loss functions:

$$\text{MSE} = \frac{1}{n} \sum_{j=1}^n (y_j - \hat{y}_j)^2, \quad (\text{S1})$$

$$\text{MAE} = \frac{1}{n} \sum_{j=1}^n |y_j - \hat{y}_j|, \quad (\text{S2})$$

$$\text{MAPE} = \frac{100\%}{n} \sum_{j=1}^n \left| \frac{y_j - \hat{y}_j}{y_j} \right|, \quad (\text{S3})$$

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{j=1}^n (y_j - \hat{y}_j)^2}, \quad (\text{S4})$$

where y is the observed value and \hat{y} is the predicted value, n is the total number of the samples in a set.