

## Supplemental

### **A design methodology of crystal growth furnace and process aided by two-step optimization using machine learning models and genetic algorithm**

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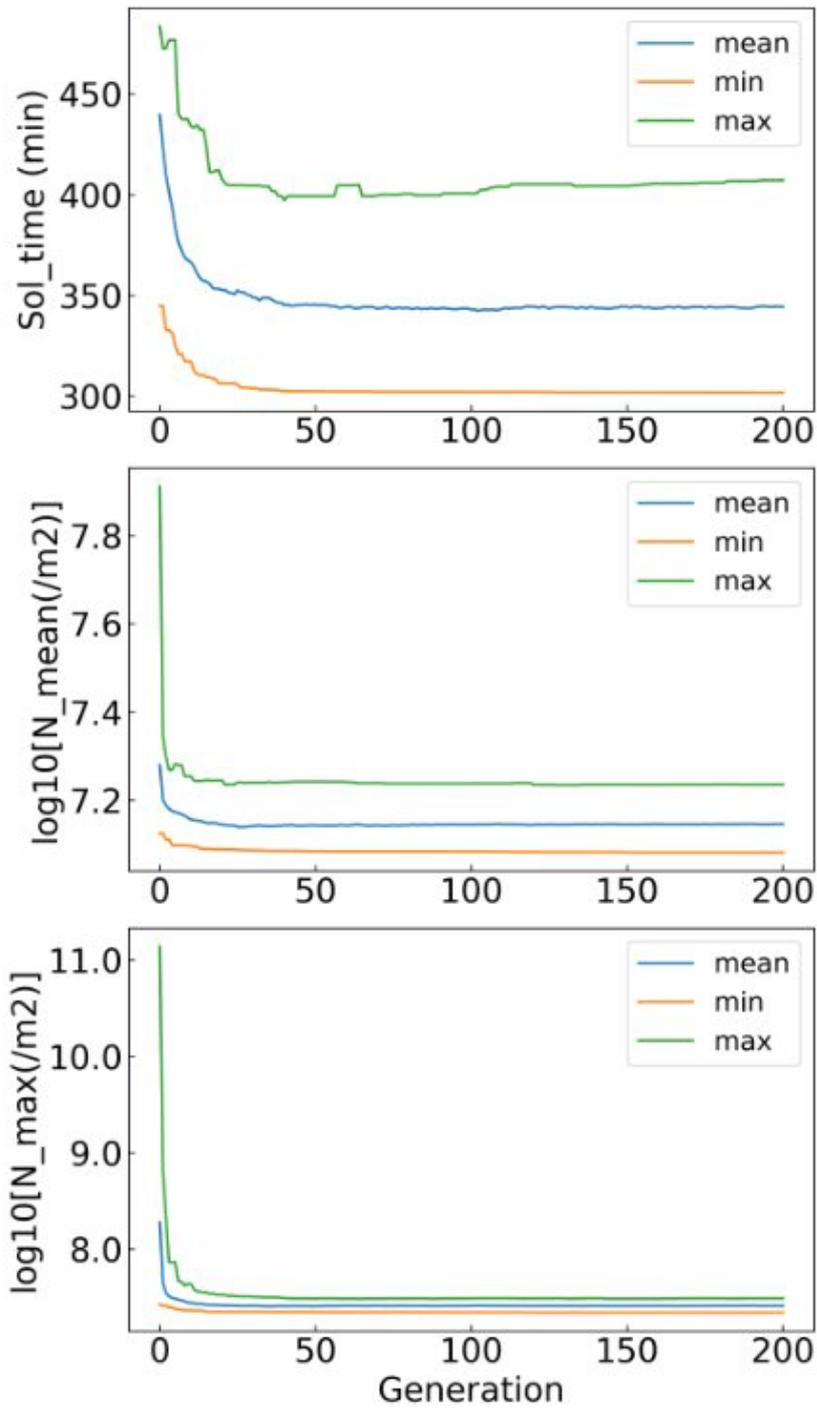
\*E-mail: [usa@material.nagoya-u.ac.jp](mailto:usa@material.nagoya-u.ac.jp)

**Table S1. DNN accuracy of Molde A**

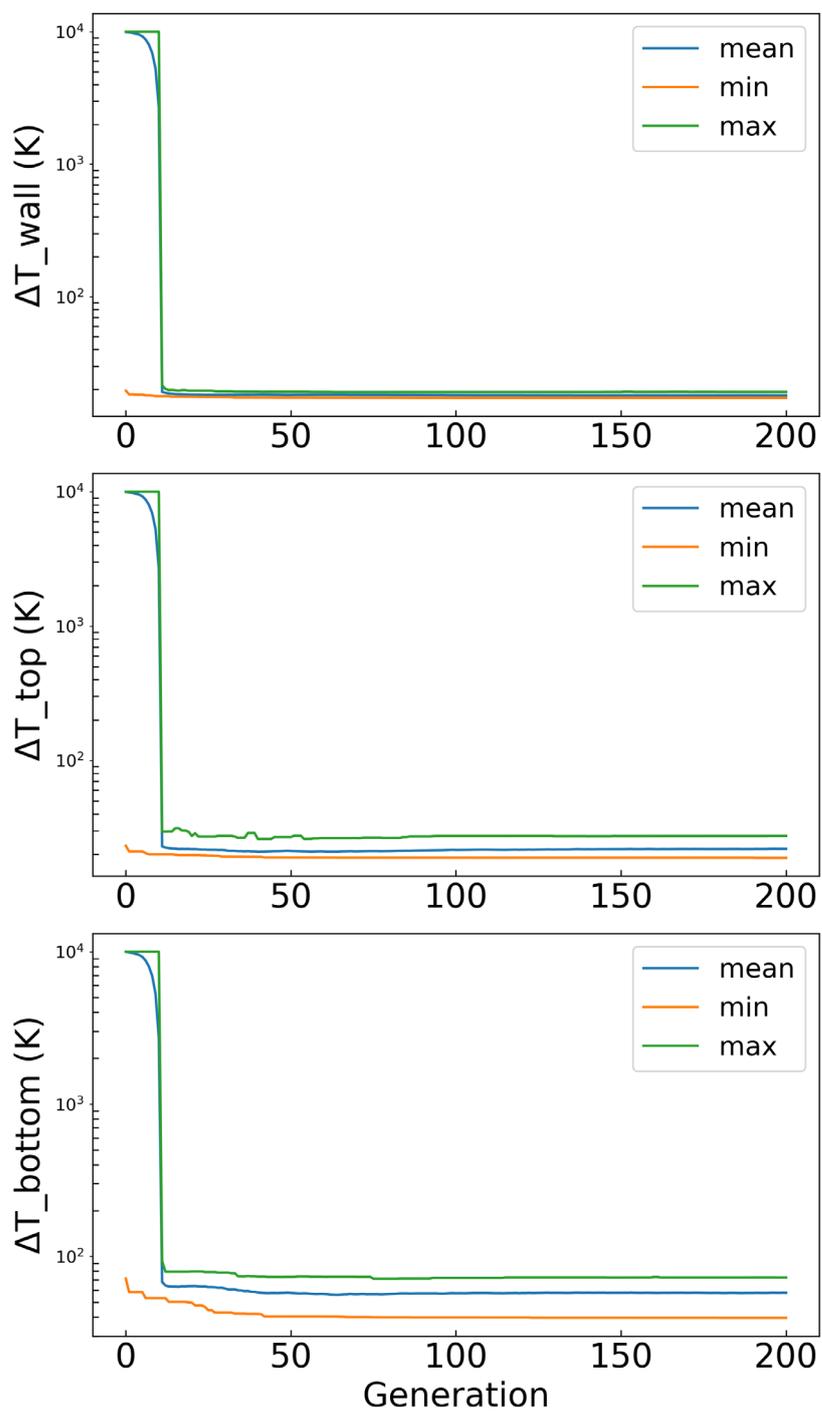
		MSE	MAE	R2
fold1 T[K]	$t$ (min)	4.639	2.769	0.998
	$\log_{10}[\text{N}/(\text{m}^2)]$	0.110	0.059	0.872
fold2 T[K]	$t$ (min)	4.347	2.707	0.998
	$\log_{10}[\text{N}/(\text{m}^2)]$	0.066	0.037	0.944
fold3 T[K]	$t$ (min)	6.416	3.533	0.996
	$\log_{10}[\text{N}/(\text{m}^2)]$	0.125	0.053	0.818
fold4 T[K]	$t$ (min)	4.918	2.663	0.997
	$\log_{10}[\text{N}/(\text{m}^2)]$	0.118	0.053	0.881
fold5 T[K]	$t$ (min)	4.473	2.843	0.998
	$\log_{10}[\text{N}/(\text{m}^2)]$	0.092	0.044	0.888

**Table S2. DNN accuracy of Molde B**

	MSE	MAE	R2
fold1 T (K)	19.012	13.224	0.793
fold2 T (K)	15.828	11.481	0.854
fold3 T (K)	19.23	14.077	0.788
fold4 T (K)	21.29	14.194	0.742
fold5 T (K)	14.638	10.902	0.862



**Figure S1.** The progress of the three objective functions in the genetic algorithm for Model A. The solution converged sufficiently within the 200 generations.



**Figure S2.** The progress of the three objective functions in the genetic algorithm for Model B. The solution converged sufficiently within the 200 generations.