The 2021 World Congress on
Advances in Structural Engineering and Mechanics (ASEM21)
GECE, Seoul, Korea, August 23-26, 2021

Materials By Design: Use Deep Generative Model

* Bor-Yann Tseng [1] and Chi-Hua Yu [2]

[1), 2)] *Department of Engineering Science, National Cheng Kung University, No. 1, University Rd., Tainan, 701, Taiwan*
[2)] *jonnyyu@gs.ncku.edu.tw*

ABSTRACT

Here we report new design approaches for various materials, such as nanocomposite materials, biomaterials, and bioinspired structural materials, using artificial intelligence (AI). AI can substantially improve the computational ability especially in multiscale modeling. We first apply a deep generative neural network to predict *crack path and fracture toughness of brittle fracture in crystalline materials*. Fracture is a catastrophic process; whose understanding is critical for evaluating the integrity and sustainability of engineering materials. However, fracture prediction in brittle materials can be difficult, especially in complex microstructures. Here we present a machine learning approach to predict fracture processes, enabling a computationally efficient way to analyze and design materials, connecting molecular simulation into a physics-based data driven multiscale model. Based on atomistic modeling and a novel image processing approach, we compile a comprehensive training data set featuring fracture patterns and toughness values for different crystal orientations. A LSTM based neural network is implemented alongside coevolutionary neural networks, designed to learn the emerging fracture patterns from the molecular modeling-based training dataset. Assessments of the predictive power of the machine learning model shows excellent agreement not only regarding the computed fracture patterns, but also the fracture toughness values, and is examined for both mode I and mode II loading conditions. We further examine the ability of predicting fracture patterns in bi-crystalline materials and material with gradients of microstructural crystal orientation. These results further underscore the excellent predictive power of our model. Looking ahead, out model could easily be scaled up and extended to different kinds of fracture predictions. Potential applications of this model could be in composites design, to develop high toughness materials and other materials by design applications such as surface coatings.

.

REFERENCES

C.-H.Yu, Z.Qin, and M. J.Buehler, “Artificial intelligence design algorithm for nanocomposites optimized for shear crack resistance,” *Nano Futur.*, 2019, doi: 10.1088/2399-1984/ab36f0.

K.Guo, Z.Yang, C.-H.Yu, andM. J.Buehler, “Artificial intelligence and machine learning in design of mechanical materials,” *Mater. Horizons*, 2021, doi: 10.1039/d0mh01451f

---

[1)] Graduate Student
[2)] Professor