Neural Network Molecular Dynamics Simulations on Chemical-Reaction-Induced Fracture and Wear Processes

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High fracture toughness and super-low wear have become urgent social issues to maximise the efficiency of energy use in automobiles, aircraft, industrial robots, etc. A lot of molecular dynamics simulations on fracture and wear processes at solid-liquid interfaces have been carried out using reactive force fields [1-5]. However, the complex chemical reactions of many element systems containing seven or more elements cannot be well simulated by the reactive force fields because of the combination explosion of parameter determination. Therefore, to solve the combination explosion problems of parameter determination, we focus on the neural network molecular dynamics approaches.

Recently, we have developed an in-house neural network molecular dynamics code "Laich+" [6] and successfully applied it to simulatng the complex chemical reactions of many element systems containing seven or more elements. At the conference, we will present the successful application of our neural network molecular dynamics code to simulating the chemical-reaction-induced fracuture and wear processes of the water/high-entropy alloy (Fig. 1) and lubricant/iron interfaces.

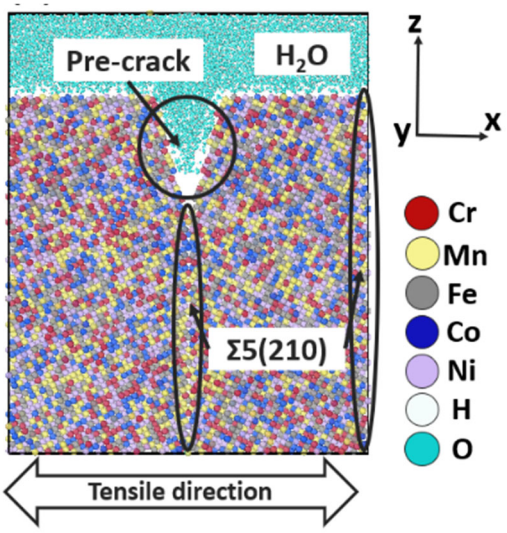

Fig. 1 Tensile simulation models of FCC-type $Cr_{20}Mn_{20}Fe_{20}Co_{20}Ni_{20}$ alloy with a pre-crack in water environments

References

1. Y. Wang, N. Yamada, J. Xu, J. Zhang, Q. Chen, Y. Ootani, Y. Higuchi, N. Ozawa, M.-I. De Barros Bouchet, J. M. Martin, S. Mori, K. Adachi, and M. Kubo, *Sci. Adv.*, **2019**, 5, eaax9301.
2. Y. Wang, J. Xu, Y. Ootani, N. Ozawa, K. Adachi, and M. Kubo, *Adv. Sci.*, **2021**, 8, 2002827.
3. Q. Chen, J. Xu, Y. Su, S. Uehara, S. Bai, Y. Wang, Y. Ootani, N. Ozawa, and M. Kubo, *Comp. Mater. Sci.*, **2022**, 208, 11354.
4. Y. Wang, H. Zhao, C. Liu, Y. Ootani, N. Ozawa, and M. Kubo, *RSC Adv.* , **2023**, *13*, 6630-6636.
5. J. Zhang, Y. Wang, Q. Chen, Y. Su, S. Bai, Y. Ootani, N. Ozawa, K. Adachi, and M. Kubo, *Carbon*, **2025**, 231, 119713.
6. R. Kudo, Y. Ootani, S. Fukushima, N. Ozawa, and M. Kubo, *Chem. Lett.*, **2024**, 53, upae114.