Neural network kinetics: exploring diffusion multiplicity and chemical ordering in compositionally complex materials

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Abstract

Diffusion involving atom transport from one location to another governs many important processes and behaviors, such as precipitation and phase nucleation. The inherent chemical complexity in compositionally complex materials poses challenges for modeling atomic diffusion and the resulting formation of chemically ordered structures. Here, we introduce a neural network kinetics (NNK) scheme [1] that predicts and simulates diffusion-induced chemical and structural evolution in complex concentrated chemical environments. The framework is grounded on an efficient on-lattice structure and chemistry representation combined with artificial neural networks, enabling precise prediction of all path-dependent migration barriers and individual atom jumps (Figure 1). To demonstrate the method, we study the temperature-dependent local chemical ordering in a refractory NbMoTa alloy and reveal a critical temperature at which the B2 order reaches a maximum (Figure 2). The atomic jump randomness map exhibits the highest diffusion heterogeneity (multiplicity) in the vicinity of this characteristic temperature, which is closely related to chemical ordering and B2 structure formation. The scalable NNK framework provides a promising new avenue to exploring diffusion-related properties in the vast compositional space within which extraordinary properties are hidden.

Using the NNK, we study vacancy diffusion in NbMoTa alloy across a broad temperature range from 2600 to 800 K [2]. Unlike pure metals, the two key diffusion parameters, diffusion correlation factor and activation energy, are not constant in alloys, but instead substantially decrease with decreasing temperature. This temperature dependence arises from a reduced number of active vacancy jump pathways at lower temperatures, leading to more correlated diffusion. Upon examining vacancy diffusion throughout the entire compositional space of the Nb-Mo-Ta system, we discover that the slowest vacancy diffusion surprisingly occurs in the non-equimolar region, rather than the equimolar concentration, where the configurational entropy is highest. The diffusion barrier spectrum, characterizing the diffusion energy landscape, is an intrinsic material characteristic that controls the diffusivity. Finally, we find that the vacancy diffusion rate drops noticeably in the presence of local chemical order in the NbMoTa system, particularly for MoTa alloys with long-range B2 order.

References

[1] B Xing, T. Rupert, X. Pan, and P Cao. "Neural network kinetics for exploring diffusion multiplicity and chemical ordering in compositionally complex materials." ***Nature Communications*** 15, no. 1 (2024): 3879.
[2] B. Xing, W. Zou, T. Rupert, and Penghui Cao. "Vacancy diffusion barrier spectrum and diffusion correlation in multicomponent alloys." ***Acta Materialia*** 266 (2024): 119653.

Figures

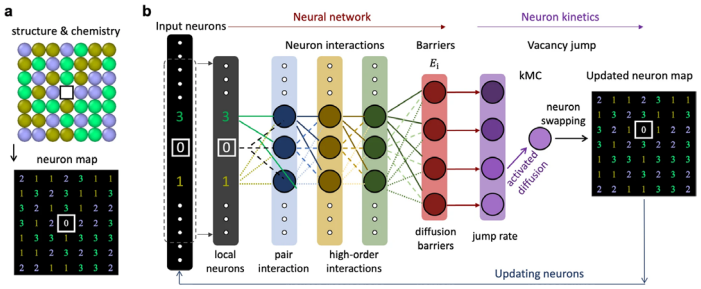

Figure 1. Schematic illustration of neural network kinetics (NNK) framework.

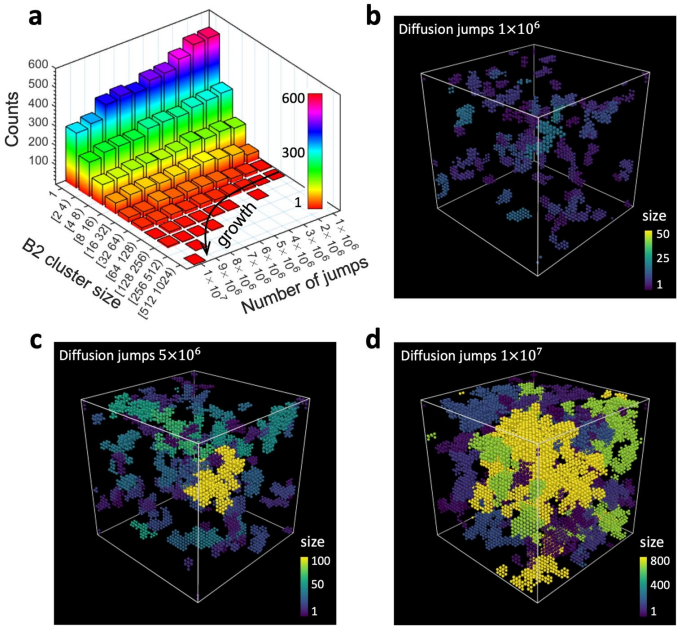

Figure 2. B2 structure nucleation and growth kinetics during annealing in NbMoTa.