

PROCEEDINGS

Inductive and Deductive Scale-Bridging In Hierarchical Multiscale Models for Dislocation Pattern Formation in Metal Fatigue

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ABSTRACT

Fatigue fracture accounts for a substantial fraction of failure cases in industrial products, especially in metal materials. While the mechanism of fatigue crack propagation can be understood in the mechanical point of view considering the effect of microstructures and crystal orientations on crack growth, there is still much room for investigations of the mechanism of fatigue crack formation under cyclic loading. It is widely understood that the fatigue crack formation in macroscopic metal materials originates in the persistent slip band (PSB) formed as a result of self-organization of dislocation structures [1]. Nevertheless, the PSB formation mechanisms proposed thus far have room for further examination and assessment, urging investigation by modeling and simulation. Moreover, recent experimental studies of fatigue in nanometer- or submicron-sized materials by Sumigawa et al. [2,3] indicate the possibility of unveiled mechanisms of fatigue at the nanometer and submicron scales, or “nano-micro fatigue”, emphasizing the importance of revealing mechanisms of dislocation pattern formation as a precursor of fatigue crack nucleation.

The reaction-diffusion model proposed by Walgraef and Aifantis [4] is widely used to simulate the dislocation structure formation. The model efficiently realizes the development of immobile and mobile dislocation densities, which occurs as a result of dislocation self-diffusion and interaction (trapping, annihilation, etc.) between dislocations. A challenge in the approach is, however, the difficulty in the determination of appropriate parameters in the governing equations because deductive (bottom-up) determination for such a phenomenological model is problematic.

As a solution to this problem, we propose an inductive approach with the machine-learning method to search a WA-model parameter set that produces simulation results consistent with experiments [5]. Using a thin film model, we performed numerical simulations for various sets of input parameters to obtain dislocation patterns. The resulting patterns were represented by the following two parameters; the number of dislocation walls, and the average width of the walls. Then, we constructed an artificial neural network (ANN) model to map between the input parameters and the output dislocation patterns. The constructed ANN model successfully predicted dislocation patterns. The presented scheme of inductive determination of simulation model parameters can be regarded as a top-down approach to find an appropriate constitutive laws of materials.

Moreover, we also propose statistical atomistic models to determine the WA-model parameters in a deductive manner. For example, self-diffusion of dislocations can be described as a probabilistic problem where dislocations moving forward and backward under cyclic shear strains are chosen randomly. In addition, the probability of dislocation trapping can be obtained by stochastic calculation of energy gain (or loss) by introduction of a dislocation in a dislocation forest.

The combination of the proposed deductive and inductive determinations of simulation parameters makes it possible to remarkably improve the credibility of the estimated parameters. This approach provides a new scheme to bridge models for different length scales, which we call DIMS (deduction-induction integrated multiscale simulation).



KEYWORDS

Reaction–diffusion model; Dislocation structure; Fatigue; Artificial neural network; Multiscale simulation; Machine learning

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