Prediction of fatigue crack initiation has presented engineers with a challenging problem over the years. Classically, predictions are based on a statistical regression of test data. Reducing the necessary certification testing and pushing the envelope of our design allowables has led to a great interest in linking the microstructure of the material to fatigue properties and life prediction.

In this presentation, we discuss a model that integrates results of atomic simulations to the continuum level. Our approach is to model the energy of a persistent slip band (PSB) structure and use its stability with respect to dislocation motion as our failure criterion for fatigue crack initiation. Through this methodology, the fatigue life is predicted based on the energy of the PSB, which inherently accounts for the microstructure of the material. Very good agreement is shown between the model predictions and an ensemble of experimental test data. Further efforts for model validation are shown, including how this type of modeling fits within an integrated computational materials science and engineering framework.