Statistical Modeling of Thermally Activated Phenomena in Discrete Dislocation Dynamics

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Thermally activated phenomena such as self-diffusion, dislocation climb and cross-slip play an important role in the inelastic deformation of metals. The strain rate sensitivity of plastic flow and the rates of creep and recovery at elevated temperatures are controlled by the energetics of dislocation interactions with obstacles. Here, we present an algorithm for thermally activated motion of discrete dislocations through a random field of obstacles using the statics of individual activation events and the kinetic Monte Carlo (kMC) method. The algorithm is illustrated using simulations of creep in single crystals at elevated temperatures. A plane strain model of a bulk single crystal subjected to constant average stress is simulated using a periodic representative volume element and the two dimensional dislocation dynamics model of Van der Giessen and Needleman (1995). It is assumed that the rate controlling process for creep is diffusion mediated climb of dislocations over local obstacles by the formation of double jogs. The rates of dislocation activation events, estimated using approximate analytical models of dislocation climb due to bulk and pipe diffusion of vacancies, are used as input to the kMC algorithm to compute the time evolution of the overall strain. It is shown that the resulting model reproduces realistic creep rates at various homologous temperatures and the experimentally observed values of the stress exponent for 'power-law' creep. Some results for creep damage evolution in single crystals will also be shown using the new method.