

A better understanding of the physics of entropy generation at multiple length scales (micro--to macroscale) during fatigue damage may provide more insight into the stochastic nature of fatigue failure. An accurate evaluation of entropy generation at multiple length scales might therefore shed more light on the physics of fatigue crack initiation. Since entropy generation is an additive function, the total entropy generation can be presented as the sum of entropy changes associated with the material and process at corresponding scale levels: $dS_{tot} = dS_{micro} + dS_{meso} + dS_{macro}$ (2) where S_{tot} = total entropy generation of the system under study; S_{micro} = entropy generation at microscale; S_{meso} = entropy generation at mesoscale; and S_{macro} = entropy at macroscale. As a consequence of the ongoing cyclic slip process, the Persistent Slip Bands (PSBs) evolve and interact with high-angle Grain Boundaries (GBs), the result of which leads to dislocation pile-ups, static extrusions in the form of ledges/steps at the GB, stress concentration, and ultimately crack initiation. We present entropy generation of dislocation activities to find answers for some fundamental questions: whether fatigue damage is a submartingale or strictly increasing function with time; whether entropy, instead of its counterpart, energy function, provides additional insights into our understanding of fatigue damage evolution; and whether entropy can be used in a fundamental way to predict the evolution of damage enabling fatigue life predictions. Regarding fatigue, damage may be defined as a reduction in the Young's modulus, as a cumulative number of cycles ratio, as a reduction of load-carrying capacity, as crack length, or as released strain energy (Amiri & Modarres 2014.) In this paper, we consider fatigue damage as slip irreversibilities that exist in a material and accumulate during fatigue loading.

3 Entropy as damage metric

3.1 Various forms of degradation

The Degradation-Entropy Generation (DEG) theorem developed by Bryant et al. (2008) states that the rate of degradation is related to the irreversible entropy generations by the underlying dissipative physical processes that degrade materials. That is, a structural transformation takes place in the dislocation ensemble upon crack initiation such that randomly-distributed-dislocation density reduces due to self-organization and the formation of the patterned planar-dislocation wall structure or microcracks. This criterion known as Lyapunov's theory of stability may provide a crack initiation criterion based on the entropy of the system by defining a control parameter x which is changing from equilibrium state A to equilibrium state B. Control parameter x is defined in the context of statistical thermodynamics by Jarzynski (2011). However, the formation of the patterned planar-dislocation-wall structures at microscale and submicron may be considered as the configuration entropy that decreases and results in increased orderliness of the system, i.e. $dS_{micro} < 0$. Ostoja-Starzewski & Malyarenko (2014) use the Doob-Meyer decomposition which says that under mild technical conditions any submartingale is the sum of a martingale (M) and an increasing process (G). This concept has been stabilised within the context of statistical mechanics which indicated that the deterministic nature of non-decreasing dissipation function is the average manifestation of a statistically fluctuating dissipation on very small scales. As mentioned above, in calculation of entropy, it is of paramount importance to consider behavior of entropy evolution at multiple length scales, because entropy generation at small scales is a stochastic phenomenon with possible deviation from the second law of thermodynamics. Amiri & Modarres (2014) have invoked this hypothesis and have shown that the rate of damage in various processes such as fatigue, wear, corrosion, radiation damage and creep can

be evaluated based on the rate of entropy generation. Stewart et al. (2006) employed non-equilibrium thermodynamics theory to predict the initiation of dynamic recrystallisation (DRX) for nickel and steels.

3.3 Fatigue crack initiation

As mentioned earlier, it is widely accepted that strain localization due to increasing dislocation density during cyclic forward and reverse loading is a precursor to fatigue crack initiation. Equation (2) suggests that even if bulk stress and strain are in the elastic range, the vicinity of inherent micro defects deformation can be locally plastic. From definition of Gibbs free energy and its relation to entropy of the system $G = H - TS$, where H is enthalpy, T is temperature and S is entropy, we will derive the necessary entropic condition for crack initiation based on instability criterion of the system:

However, the decrease of entropy and increase of orderliness at microscale is compensated by the entropy increase at the mesoscale due to the formation and propagation of cracks, i.e. $dS_{meso} > 0$. τ_0 is the fatigue nucleation life associated with virtual crack length a . Mathematically, to maximize the Gibbs free energy, one can write: $dG/da > 0$. The in situ neutron diffraction study by Huang et al. (2010) states that dislocation self-organization arises possibly during the formation of a microcrack.

2.1 Entropy balance at multiple length scales

Let us confine our discussion to length scale that spans from micro to macro. In an open system capable of exchanging heat and matter with its surroundings the change of the total entropy, dS consists of sum of two parts: $dS = dS(e) + dS(i)$; (1) where $dS(e)$ is the entropy exchange with the surroundings (or reversible entropy change) and $dS(i)$ is the entropy generation within the system (or irreversible entropy change). This suggests that even if bulk material undergoes a reversible process, at lower scales it might experience irreversibilities that are not observed at continuum level. This theorem states that there is one-to-one correspondence between the rate of entropy generation and the rate of degradation relating to each other through a scaling factor called degradation coefficient. As outlined in the previous section, the entropy generation is a submartingale meaning that at small scales the entropy generation can become negative that gives rise to behavior not seen under the restriction of the conventional second law of thermodynamics. As discussed by Mughrabi (2009), the mechanisms of cyclic microplasticity, based on the glide of dislocations, are responsible for the fatigue phenomena. In fact, cyclic slip irreversibilities in a microstructural sense occur not only at the surface but also in the bulk at the dislocation scale which contribute to surface fatigue damage. Employing non-equilibrium thermodynamics, we may develop the necessary formulations for evaluations of entropy generation during fatigue damage. The rate of entropy generation due to dislocations activities can be expressed as (Huang et al. 2009): $dS/dt = \dots$. As stated earlier, if a nonequilibrium stationary system loses its stability, the excess entropy should satisfy $dS/dt > 0$. (the inequality in (7)). Therefore, $dS/dt > 0$.