Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E1]Poster Session 1

Symposium E

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-24]Molecular Dynamics Simulations of Low-cycle Fatigue Behavior in Single Layer Molybdenum Disulfide

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Graphene-like two-dimensional transition metal dichalcogenides (TMDs) have attracted much interest in the last decade because of it astonishing properties. Molybdenum disulfide (MoS2) is one of TMDs. It has direct band gap of 1.8 eV in monolayer but its bandgap can change with the number of layers. Such properties make it industrial important. In order to ensure the reliability of nano-devices made by MoS2, much attention has been focused on their mechanical properties including elastic modulus, stiffness and breaking strength. However, only limited studies have been done on cyclic deformation and fracture behavior. As a result, we report on molecular dynamics simulations of low-cycle fatigue behavior in single layer molybdenum disulfide. We choose the Reactive Empirical Bond Order (REBO) potential to describe the interatomic interactions. The REBO potential is used to estimate the failure strain and the tensile strength. The simulations and subsequent analysis suggest that the tensile stress will make the vacancies penetrate the whole plane, and induce the fracture for incremental brittle crack growth to occur during near-threshold fatigue. We want to clarify whether the plastic-strain-controlled fatigue tests would show the Coffin-Manson relation in fatigue life. Such power-law form originates from plastic-strain-dependent microscopic damage accumulation. Lastly, the effect of a crack on low-cycle fatigue of monolayer MoS2 in terms of failure mode and fatigue life is also discussed.