GRADUATE STUDENT RESEARCH SEMINAR SERIES (2020)

PHASE TRANSITION OF MOS2 UNDER EXTERNAL LOADING: A MOLECULAR DYNAMICS STUDY

SPEAKER: MAHABUBUR RAHMAN

Two-dimensional Transition Metal Dichalcogenide (TMD) materials have started to find their applications on electrical, thermal devices. For example, MoS2 from single layer to few layers has been used in electrical devices due to its semiconducting nature that overcomes the shortcomings of graphene and has the potential of replacing Si as semiconductor. TMD's has higher degree of freedom in out-of-the plane direction as compared to graphene leading to possible phase transformation under the influence of external forces. Since electrical and thermal devices fabricated using MoS2 varies from few nanometers to micrometers, the devices are susceptible to edge effect and as a result the phase transition of MoS2 can alter its material behaviors. So far, there are some phase (2H phase is common), 1T, 1T`, 1T`` phases have been found to be stable at room temperature, experimentally and computationally. These phases have already proved to alter the mechanical and thermal properties e.g. the 1T` phase has higher elastic modulus then 2H phase. In this work, phase transition in bilayer MoS2 (BLMoS2) under tensile loading is explored through systematical molecular dynamics (MD) simulations. The quadrilateral phase is observed on monolayer and bilayer of MoS2 under uniaxial tension in ArmChair (AC) and ZigZag (ZZ) directions. The quadrilateral phase leads strain hardening at 34 percent strain in AC direction tension test. Such strain hardening effect gives higher energy absorption capability as compared to the single layer 2H MoS2. Most recently, synthesized Sulphur line vacancy has been reported on the surface of the bulk and few layers of MoS2 using hydrothermal process that found to be stable up to 90% vacancy. The direction and width of the S line vacancy to the phase transition of BLMoS2 has been systemically investigated under the uniaxial tensile test in the armchair direction. The density increase of Sulphur vacancy advances the quadrilateral phase transition process at a smaller strain in AC direction, comparing to the pristine BLMoS2 case. With 10% Sulphur line vacancy in the AC direction, the original honeycomb structure of BLMoS2 lattice cannot be maintained.

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