TEMPLE UNIVERSITY
Department of Mathematics

Applied Mathematics and Scientific Computing Seminar

Wednesday, 12 September 2018, 4:00 p.m.
Room 617 Wachman Hall

(refreshments and social at 3:45 p.m)

A Reactive Molecular Dynamics Study of Graphene as a Protective Barrier Against Hydrogen Embrittlement

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Abstract. Hydrogen is highly mobile and can diffuse through metals very easily. Hydrogen dissolved in metals and alloys can induce catastrophic failure at markedly lower load levels compared with those of hydrogen-free materials; this phenomenon is known as hydrogen embrittlement (HE). The damage caused by HE is normally invisible and unforeseeable, and failure can occur without warning. Therefore, HE failure is much more dangerous than other types of fastener failure. One recent high-profile incident caused by HE occurred during the construction of the new east span of the San FranciscoOakland Bay Bridge in California, USA. Although several major mechanisms of HE have been proposed, including hydrogen-enhanced decohesion, adsorption-induced dislocation emission/void coalescence, and hydrogen-enhanced localized plasticity, uncertainty over the mechanism of HE remains. Many methods have been proposed to prevent HE, including heat treatment and formation of a protective barrier of zirconium dioxide or polyaniline nanofibers. However, none of these methods are effective enough. Therefore, an advanced method to prevent HE is required. Some research has suggested that the permeability of hydrogen can be decreased by using a diamond-like carbon thin film coating. Graphene is a two-dimensional

single-atom-thick sheet of carbon, and it has extraordinary physical, chemical, and mechanical properties. A perfect single layer of graphene is impermeable to standard gases including helium, and graphene can act as a barrier to prevent the oxide formation on a protected metal. Motivated by these properties, we considered that graphene could be an ideal material for use as a hydrogen protection barrier to protect metals from HE damage. In this work, reactive molecular dynamics simulations were performed to investigate the hydrogen barrier performance of graphene. Reactive molecular dynamics using the ReaxFF force field, which can simulate the formation and breaking of bonds, was used to model chemical reactions. The reactive molecular dynamics has almost the same level of accuracy as that of first-principles calculations but at much lower computational cost. Because it is usually difficult to form large-scale uniform graphene in practical experiments, the effect of a defect on the gas barrier performance was investigated as compared with a perfect graphene sheet.