

PhD Dissertation Defense Announcement  
Mechanical and Aerospace Engineering Department  
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**A MOLECULAR SCALE STUDY OF CAVITATION GROWTH  
AND SHOCK RESPONSE IN SOFT MATERIALS**

**By**

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**Abstract**

Cavitation is a mechanism through which small vapor-filled cavities are formed in a liquid medium due to rapid changes of pressure. In liquid, cavitation bubble is created when surrounding pressure drops below the saturation vapor pressure. Here, cavitation formation due to shock wave is considered. The molecular level heterogeneous and homogenous cavitation mechanisms and bubble growth kinetics in soft gelatin hydrogel and water has been studied. Gelatin, which is derived from collagen, is frequently used as a brain simulant material. As such, morphology of gelatin is very different from water. In the heterogeneous cavitation study, using molecular dynamics simulation, the pressure requirement for a nanoscale cavitation to grow in water and gel has been investigated. The results show that a gel-like structure requires higher pressure for the cavitation to grow, and both gel and water models exhibit strain rate effect on the cavitation threshold pressure. The results also suggests that the cavitation collapse time is

dominated by the viscosity of the medium. In homogeneous cavitation study, the same models in the absence of preexisting bubble is stretched by volume controlled stretching at six different strain rates. It is quite interesting to note that while critical tensile pressure for homogenous bubble nucleation of gel like model is higher than the water at lower strain rates, at higher strain rate the critical pressure is quite similar, thus empirical relation cannot be obtained at much higher strain rate. The cavitation formation rate governs by the viscosity of the medium. In the second part of the study, ECM components such as Perineuronal net (PNN) which is one of the most prevalent component that surrounds the neuronal cell has been used to analyze the mechanics under shock loading. Assessment of the damage efficiency of the PNN molecules at different conditions such as shock speed, preexisting bubble and boundary conditions have been considered. The change of the bonding morphology which is responsible for the stability of the secondary structure of the protein molecules of the PNN has been analyzed to evaluate the damage level.