TEXAS A&M UNIVERSITY at QATAR

Chemical Engineering Program

First Principles Method in Studying Stress Corrosion Cracking in Metals

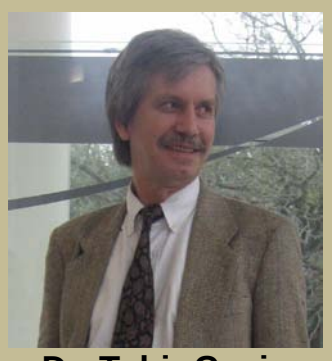
Dr. Tahir Cagin

April 09, 12-01PM

Lecture Hall 238

(Light Lunch will be served)

Stress corrosion cracking in metals in particular in iron and iron based alloys is critical to material failure for many of their applications. In this presentation, we will present a description of processes leading to these failures and review some predictive methods employed in studying these processes. We present our recent studies using density functional theory to study the behavior of Ni and Fe Σ3(111) grain boundary (GB) under precipitations of S, P, N, C and B to elucidate their stress corrosion effects, as well as its mechanisms. There are certain locations that that impurities have more tendency to segregate. Some elements such as C and B serve as strengtheners while S, P and N weaken the Fe-Fe interactions at GB. However, the stress corrosion failures arise in a variety of ways. The accumulation of S and P results in separation of grains; this in turn gives rise to the inter-granular cracking under sufficient stress.



Dr. Tahir Cagin

He is currently holding Professorship at Chemical Engineering, and Materials Science programs (served as Chair between 2008-2010 and serving as the executive committee member) at Texas A&M University. He is also serving as the member of graduate faculty for the Mechanical Engineering Department. He is a well-known expert in modeling and simulation of nanomaterials for a wide range of applications. For his work in nanotechnology he was awarded the Feynman Prize in Nanotechnology in 1999. Dr. Cagin is born in Izmir, Turkey, where he received basic and high school education. He has completed his BS and MS degree in Physics at Middle East Technical University, Ankara. He has completed his Ph. D. in Physics at Clemson University, 1988. He has spent 18 months as a postdoctoral fellow at University of Houston, Chemistry Department. After serving a year as a research associate at the Materials Laboratory of Wright Patterson AFB, he has joined Molecular Simulation Inc. (Presently Accelrys) where he has spent around four years as senior research and development scientist, product manager and research director. In the summer of 1995, he has joined Caltech, Materials and Process Simulation Center, as senior research scientist. He has moved to Texas A&M University in 2005 as a professor of Chemical Engineering. Over the last 20 years he has developed and applied multi scale simulation methods into various materials science and engineering problems; such as the material behavior under extreme environmental conditions through various stages leading to material failure (stress corrosion, metal dusting, etc.). His notable research is in the area of nano science and nanotechnology areas with a particular focus on the materials for energy harvesting, conversion and storage (thermoelectrics, photovoltaics, piezoelectrics, fuel cells, supercapacitors, etc.).

FOR MORE INFORMATION:

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