MM 22: HV Paxton

Time: Tuesday 14:00–14:30 Location: H 1058

Invited Talk MM 22.1 Tue 14:00 H 1058

Grain boundary embrittlement and cohesion enhancement in copper — •Anthony Paxton[1], Alexander Lozovoi[1], Rainer Schweinfest[2], and Michael Finnis[3] — [1]Atomistic Simulation Centre, Queen's University Belfast, BT7 1NN, UK — [2]Science+Computing ag, Hagellocher Weg 71-5, 720270 Tübingen, Germany — [3]Imperial College London, Exhibition Road, London SW7 2AZ, UK

There has been a long standing debate surrounding the *mechanism* of grain boundary embrittlement and cohesion enhancement in metals. Embrittlement can lead to catastrophic failure such as happened in the Hinkley Point disaster, or indeed in the case of the Titanic! This kind of embrittlement is caused by segregation of low solubility impurities to grain boundaries. While the accepted wisdom is that this is a phenomenon driven by *electronic* or *chemical* factors, using language such as *charge transfer* and *electronegativity difference*; we believe that in copper, at least, both cohesion enhancement and reduction are caused by a simple *size effect*. We have developed a theory that allows us to separate unambiguously, if not uniquely, chemical and structural factors. We have studied a large number of solutes in copper using first principles atomistic simulation to support this argument, and the results of these calculations will be presented here