8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

ELECTRONIC-STRUCTURE CALCULATIONS AT MACROSCOPIC SCALES

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ABSTRACT

Density-functional theory (DFT) has provided valuable insights into materials structure and properties at the nanoscale. However, its computational complexity has kept macroscale properties, especially those involving defects, beyond reach. Multiscale analysis offers an avenue for overcoming the size constraints of conventional DFT and enabling electronic calculations of multi-million atom clusters free of spurious physics or restrictions on geometry. The key tools that make this extension possible are: i) a real-space formulation of DFT; ii) a multigrid finite-element discretization the real-space formulation; and iii) and a quasi-continuum reduction for effecting a seamless transition to the continuum. We demonstrate the application of these tools, their accuracy at affordable computational cost and the physical insights they offer by studying vacancy systems in million-atom aluminum clusters. In particular we study: the formation of prismatic dislocation loops, an important ageing mechanism in heavily irradiated nuclear reactor materials; and the formation of nanovoids under high tensile pressure, an important mechanism of void nucleation in shocked metals.