Computer model predicts how materials meet in the middle

March 16 2010, By Colin Smith and Lucy Goodchild

(PhysOrg.com) -- Predicting the way different materials fuse together at an atomic level in objects including iPods, computer chips and even ships may be possible using a new computer model, described in the March issue of *Nature Materials*.

The authors of the study, from Imperial College London, say their new approach could help engineers understand and work out in advance how materials might behave. This could help them to design better materials with improved properties such as strength, flexibility or conductivity.

When two different crystalline materials, such as metals or ceramics, are joined together, there is an interface between them where individual

atoms have to arrange themselves into certain positions. The chemical composition of this interfacial region may also be different from that of either crystal. The structure and composition of the interface can have a significant impact on the overall properties of the material.

In this video, the researchers behind the new model, Professor Adrian Sutton, from the Department of Physics, and Professor Mike Finnis, from the Departments of Materials and Physics, talk about interfaces, the computational approach they have developed and why this is a major breakthrough in materials research.

More information: "A genetic algorithm for predicting the structures of interfaces in multicomponent systems" *Nature Materials*, corrected online 4 March 2010. Corresponding author: Professor Adrian Sutton, Imperial College London. A link to the paper is available here.

Provided by Imperial College London

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