Modeling and simulation in Materials Science

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Important advances in multi-scale computer simulation techniques for computational materials science have been made in the last decade as scientists and engineers strive to imbue continuum-based models with more-realistic details at quantum and atomistic scales Materials modelling and simulation aims to develop fundamental relationships between the atomic structure and properties of molecules and materials. Simulation modelling has been used in a wide range of physical and social sciences and engineering fields, ranging from nuclear fusion to economic forecast to space shuttle design. For different types of situations and systems, different types of models are used. In classifying simulations, there are important distinctions among the types of models that are being simulated, and among the types of program structures that are used to carry out the simulation. Computer modelling and simulation are known to aid design of new materials, processes and products. A model is a conceptual description of an entity or a phenomenon, quantified using the relevant laws of science with allowable approximations and simplifications. The four important sequential steps involved in any modelling are conceptualization, simplification, representation and finally quantification. Essentially, a model provides the basis for simulation to create an image of a real system or a phenomenon. Modern computers have made simulation attractive to the extent that 'virtual reality' has become possible. Sound numerical simulations are almost equivalent to performing real experiments and therefore referred to as 'numerical experiments'. A real experiment is a direct dialogue with the system of interest and therefore expected to be naturally reliable.

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