On modelling complex crystal structures.

Toby D. Young Feburary 14, 2006

abstract

In this short talk we present an overview of our research objectives to contribute to the work of PARSEM. First we provide a résumé of multi-scale modelling of atomic structures in self-equilibrium. Secondly, we describe our direction for studying theoretical issues surrounding alloy fluctuations, random disorder and interfacial phenomena based on experimental evidence. In particular, we suggest a pathway toward modelling such features in complex crystal structures; say, for example, ternary and quaternary nitrates. Finally we tentatively address some of the known difficulties associated with our reseaerch objectives, namely, those that are to be surmounted in the near future.