

Atomic Scale Simulations for Waste Form Applications

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Abstract

A major concern at the current time is the long term storage and the eventual disposal of radioactive waste. The aim of this thesis is, by the use of computer simulation techniques, to examine various topics relating to nuclear waste disposal. These topics include simulation of a possible wastefrom material based on the pyrochlore structure, in order to determine: the relative solubilities of uranium and plutonium and also its stability with respect to the related fluorite and δ -phase structures. The results from these are presented in the form of composition maps which facilitates the identification of regions of greatest stability.

Once a waste form has been made, it is important to consider how it becomes damaged associated with to the decay processes of the radioactive species it contains. Molecular Dynamics were used to compare collision cascade events simulating α -recoils for the simple ceramic systems of pure and impure (doped with 0.2% Al) magnesium oxide. Analysis of the resulting cascade simulations showed that the anisotropy associated the direction of the damage profile was totally changed through the addition of impurities.

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