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Joint ICTP-IAEA Workshop on Physics of Radiation Effect and its Simulation for Non-Metallic Condensed Matter | (smr 2359)

Thursday 23 August 2012

Application of molecular dynamics and long time scale atomistic methods to radiation simulations in non-metallic condensed matter - Adriatico Guest House Giambiagi Lecture Hall (15:00-16:00)

The methods described in Lectures 1 and 2 will be applied to the study of radiation damage in MgO, Er2O3 and magnesium aluminate spinel, initiated by keV energy knock-on atoms. The structure of the collision cascades in these materials will be described along with some non-intuitive results concerning the diffusion of defect clusters and how the diffusion mechanisms can be further used in rate theory models.
In addition variable charge potentials will be implemented to show how oxide coatings (TIO2 and ZnO) behave when subjected to bombardment by energetic atoms, especially how the growth processes in a magnetron device occur over realistic time scales and how it is possible to use the simulation techniques to inform experimentalists of the conditions required for optimal crystalline growth.

time	title	presenter
15:00	Application of molecular dynamics and long time scale atomistic methods to radiation simulations in non-metallic condensed matter	ROGER SMITH