Table of contents

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

Tuesday 21 August 2012

Combination of experimental tools and computer modelling for investigation of radiation damage - fusion applications - Adriatico Guest House Giambiagi Lecture Hall (15:00-16:00)

Using presently available scientific concepts, modelling tools based on existing and new mathematical algorithms and computer facilities have been developed over the last decades. To guarantee robustness, models must be grounded in physics and, as far as feasible, at the scales where the latter is most fully ascertained, this often being – though not invariably so – that of the atom, the more so since irradiation damage generation and evolution mechanisms are precisely induced at this scale.

Ab-initio computation of electronic structures allows the basic properties (structure, formation, migration) of point defects to be arrived at. This has made possible the full modeling of self-diffusion, as of the crucial effects of impurities. Molecular dynamics is the basic tool for the investigation of ballistic damage processes, however its effectiveness is dependent on the quality of the interatomic potentials used. As regards insulators, moreover, the ab-initio approach, i.e. an approach based on rigorously taking into account the quantum character exhibited by physics at the atomic scale, is indispensable if electronic effects are to be taken on board, in particular the damage due to particles other than high-energy neutrons, electrons, and photons.

Predictions of long-term microstructural evolution kinetics, rely on already highly developed models, that have shown good performance with respect to metals, application of which to ceramics, however, is only just beginning. The understanding, and modeling of mechanical behavior are likewise far more advanced for metals than for ceramics, however the multiscale approach, starting from the atomic scale, is still barely at an initial stage.

At the same time, modeling must be closely coupled with experiment. Aside from gaining the relevant data as to behavior subsequent to neutron irradiation for the materials selected, it is indispensable to conduct a targeted experiment drive, aimed at ascertaining basic physical properties, and behaviors, and at the parametrization, and validation of the models.Thus, charged-particle irradiation – involving ions, and electrons – affords the possibility of mimicking, and analyzing, in detailed fashion, damage mechanisms in small, inactivated samples, which are thus amenable to a whole range of measurements, and observation, from the atomic scale up, both in situ, and ex situ.

time	title	presenter
15:00	Combination of experimental tools and computer modelling for investigation of radiation damage - fusion applications	SHEILA GONZALEZ