Aging in irradiated materials: First predictive model of the microstructure of irradiated iron

January 19 2005

Researchers from the CEA's Nuclear Energy Division have, for the first time, been able to make a quantitative prediction of the evolution of radiation-induced defects in a structural material. The results obtained for iron, using multi-scale simulation techniques based on the atomic scale, will help provide greater insight into material aging phenomena in existing nuclear power plants and may be applied to nuclear systems of the future. They are to be published in the *Nature Materials* journal on January 4, 2005.

The evolution kinetics of radiation-induced defects in a material has a direct impact on changes in its microstructure and consequently on its mechanical properties. This makes the quantitative prediction of this kinetics and the phenomena governing it a major challenge for the nuclear industry.

This challenge can now be taken up by intercoupling computer simulation techniques operating on different scales. This is what is meant by multi-scale simulation; the numerical results obtained on one time and space scale were taken and used as input data for modeling on the next higher scale:

- first of all, ab initio computer simulations rooted in quantum mechanics described the structure and migration of defects and defect clusters. These simulations, which call for considerable computing resources, were performed by drawing intensively on the capabilities of the CCRT (research and technology computing center) set up on the CEA's Bruyères-le-Châtel site.

- the second stage consisted in taking these elementary properties and reconstructing, on the basis of a kinetic model , the evolution of defects and their effects on the macroscopic properties of an irradiated iron sample one micron (a thousandth of a millimeter) in size, over a period of about one hour.

The simulations were compared with indirect experimental measurements . The excellent agreement obtained demonstrates the realism of this multi-scale model, which highlights the role played by the hitherto unsuspected migration of small interstitial and vacancy clusters. They challenge the interpretation of several earlier experiments and simulations and open the way for the quantitative simulation of more complex irradiated materials such as industrial steels. They will be used in interpreting the mechanical behavior of the ferritic steels used as structural materials in existing nuclear fission plants, as well as those proposed for future fusion plants.

Irradiation defects and the structural changes induced in materials

Provided that enough energy is transmitted, bombarding materials with high-energy particles can displace atoms within the crystal lattice via a ballistic collision phenomenon. As they are struck, the atoms can be displaced by several interatomic distances before stopping in the interstitial position, leaving behind them gaps known as vacancies. These elementary defects – interstitials and vacancies – are mobile. They can migrate in the material and gather into clusters that grow to form a defect microstructure. It is this microstructure that will affect certain properties of the material – particularly its mechanical properties – by interacting, for example, with dislocations.

Reference:
Nature Materials 4, 68–74 (2005)
Multiscale modelling of defect kinetics in irradiated iron
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Source: Commissariat a l'Energie Atomique (CEA)