Direct observation of radiation defects: experiment and interpretation.

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Electron microscopy is arguably the only available experimental method suitable for the direct visualization of nano-scale defect structures formed under irradiation. Images of dislocation loops and point-defect clusters in crystals are usually produced using diffraction contrast methods. For relatively large defects, a combination of dynamical imaging and image contrast simulations is required for determining the nature of visible radiation defects [1].

At the same time, density functional theory (DFT) models developed over the last decade have provided unique information about the structure of nano-scale defects produced by irradiation, including the defects that are so small that they cannot be observed in an electron microscope, and about the pathways of migration and interaction between radiation defects. DFT models, involving no experimental input parameters and being as quantitatively accurate and informative as the most advanced experimental techniques for the direct observation of defects, have created a new paradigm for the scientific investigation of radiation damage phenomena. In particular, DFT models offer new insight into the origin of temperature-dependent response of materials to irradiation, a problem of pivotal significance for applications. By combining information derived from the first-principles models for radiation defects with information derived from small-scale experimental observations it may be possible to acquire quantitative knowledge about how materials respond to irradiation and, using this knowledge, develop materials suitable for advanced applications in fission and fusion.

It now appears possible to pose the question about the development of integrated fusion power plant models, combining neutron transport calculations and microscopic models for microstructural evolution of materials, for example models for *ab initio* prediction of helium embrittlement [2]. Such models, based on scientific principles and quantitative data, and developed at low cost in comparison with the mock-up tests, offer scientific insight and make it possible to perform, in combination with experimental information derived from fission and ion-beam irradiation experiments, the preliminary assessment of power plant operating scenarios.

Defining the limits of visibility of small defect clusters and dislocation loops, and optimal diffraction conditions for electron microscope imaging, remains one of the central problems of electron microscopy of irradiated materials. Using computer image simulations based on the propagation–interpolation algorithm for solving the Howie–Basinski equations, it is possible to investigate the relation between the actual and the 'observed' size of small loops, the part played by many-beam dynamical diffraction effects, and limitations of electron microscope imaging in identifying the structure of small defects [3].

A particularly impressive and useful application of electron microscopy is given by recent *in situ* electron microscope observations, providing real-time visualization of dynamics of defects produced by ultra-high-energy electron irradiation, or showing microstructural evolution occurring under ion beam irradiation. Such observations have revolutionized our understanding of how properties of metals and alloys change in the extreme radiation and thermal environments of a fission or a fusion power plant.

The key feature of *in situ* electron microscopy is its ability to exhibit the time-dependent dynamics of migration, interaction, and transformation of radiation defects, and to visualize the entire complexity of evolving defect and dislocation networks. For example, *in situ* electron microscope observations provided evidence of violation of the Burgers vector conservation law for dislocations on the nanoscale. This gave a vital clue needed for modeling microscopic processes responsible for the formation of unusual high temperature dislocation structures in iron, and for explaining the origin of the loss of strength of ferritic-martensitic steels at high temperatures.

The development of *in situ* electron microscope techniques was partially stimulated by the application of large-scale molecular dynamics (MD) simulations to modeling mobile defects and clusters of defects (for example, nano-dislocation loops) in iron and other metals. A hypothesis stating that clusters of point defects play a significant part in microstructural evolution of irradiated materials was proposed in 1990s within the framework of the "production bias" radiation damage model. However, it is only recently that *in situ* electron microscope observations confirmed the fact that mobile and immobile clusters of point defects form an integral part of the microstructure of an irradiated material.

Somewhat surprisingly, interpreting *in situ* real-time electron microscope observations still remains genuinely problematic. The ten orders of magnitude mismatch between the nanosecond (10^{-9}s) time scale accessible to an MD simulation, and the 10–1000 s time scale of a typical *in situ* electron microscope observation, impedes meaningful quantitative analysis. The need to develop such a model has recently stimulated the development of a novel approach to modeling defect evolution in real time (Langevin dynamics [4]).

In situ electron microscope observations visualize the dynamics of microstructure corresponding to the limit of high irradiation dose rates, approaching 10-3 dpa/s (80 dpa per 24 h) for the ultrahigh-voltage electron irradiation case, and ($6x10^{-4}$ dpa s^{-1} to $8x10^{-4}$ dpa s^{-1} (50–70 dpa per 24 h) for the *in situ* ion-beam irradiation case. These dose rates are similar to the 10 dpa per 24 h to 100 dpa per 24 h range of dose rates characterizing irradiation conditions in *ex situ* ion-beam facilities. *In situ* electron microscopy and *ex situ* ion-beam irradiation experiments generate similar microstructures, corresponding to a similar range of high irradiation dose rates. These dose rates are several orders of magnitude higher than the rates associated with the irradiation environment of a fission nuclear reactor, an accelerator-driven system such as the International Fusion Materials Irradiation Facility or a fusion power plant.

The dose rate effects – somewhat surprisingly – are observed even in the very low dose rate limit, for example, dose rate effects are seen in swelling experiments performed using conventional fission reactors. This highlights the dynamic nature of microstructural evolution, and the need to understand the parameters determining this evolution, at quantitative level. The refinement of nuclear cross-section data, and the development of an integrated approach describing how materials evolve under irradiation, from the treatment of neutron scattering by atomic nuclei to the development of defect microstructures in materials, is a timely objective for fission and fusion materials research.

References

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