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Editor's summary

Second IEA fusion materials agreement workshop on modeling and experimental validation

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Abstract

The present workshop dealt both theoretically and experimentally with issues of primary damage and irradiation induced defect evolution, helium and other impurities, dislocation–defect interactions, deformation to large plastic strains and fracture. It was focused on the bcc structure (Fe, V and their alloys), but a number of presentations and discussions were centred around results in the fcc and hcp structures.

1. Primary damage and defect evolution

The improvement of the reliability of the atomistic simulations starting from the primary event calculated using molecular dynamics (MD) and followed by the use of kinetic models like the rate theory and Monte Carlo (MC) simulations were discussed. An increasing use of the ab initio methods has been made in the simulations, in which the results of the ab initio calculations are used to parameterize an empirical potential. However, for the time being, the interatomic potentials based on the embedded atom method (EAM) or the Finnis–Sinclair type remain the most used ones. The main drawback of these potentials is that the calculated forces that derive from them are isotropic. For many transition metals, with strong directional bonds, the formation, binding, dissociation and migration energies of the defects and cluster of defects calculated on the basis of the EAM may be incorrect. The proper crystal structure can be reconstructed with the bond-order potentials (BOP), which are obtained by coarse-graining the quantum-mechanical electronic structure within the chemically intuitive tight-binding framework. Despite the success of the BOP in predicting crystal structures, their use in MD requires about hundred times more CPU time than an EAM potential, so they cannot yet be extensively applied to simulate high energy cascades. It has been recognized than further development of bcc potential for Fe and V (materials relevant for fusion application) is needed within the fusion radiation damage community.

New results and data were presented that give a good picture of defect production and accumulation in copper and α-iron. The nature and quantity of defects and defect clusters directly produced in the cascade, with primary knock-on atom energies ranging up to 25 keV in copper and up to 100 keV in iron for temperatures between 100 and 900 K, were reported. For such high energy cascades, the problem of electronic losses was raised in the discussion as well as the issue of electron–phonon coupling.

Up to know, most of the MD cascade calculations were done on perfect lattices of pure metals. Studies on the role of grain boundaries (GB) and vacancy clusters acting as sinks to the motion of SIA's were presented. It was found that single interstitials and mobile clusters are absorbed by the nearby GB, while single vacancies and stacking fault tetrahedra (SFT) remain in the grain interior. The structure of the grain boundary itself remains unchanged and it is only modified by the production of several cascades in the same GB.

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The role of impurities and/or precipitates on the motion of mobile clusters was outlined. It was emphasized that the role of impurities in the defect accumulation is an intrinsic problem in the sense that the impurities can be produced during the irradiation by nuclear transmutations.

In the frame of the classical nucleation theory, the nucleation of both voids and interstitial loops from the primary clusters was addressed. A single-component nucleation theory using the Fokker–Plank equation, which considers the stochastic effects of the fluxes of mobile defects, was formulated. It was shown that at elevated temperatures the nucleation of overcritical precipitates from small subcritical nuclei is similar for voids and interstitial loops. At low sink densities, fluctuations in the rate of vacancy emission govern void nucleation.

Investigations on hcp metals were also been presented. The formation energies of self-interstitial atoms (SIA) have been calculated for the hcp-zirconium, based upon first principles electronic structure calculations.

In order to explain the electron microscope observations in Fe and ferritic–martensitic steels, the energetics and reactions between $\langle 1\,1\,1\rangle$ crowdions were described and a possible explanation for the observed formation of [1 0 0] loops in iron has been put forward.

In order to extend the time span of the few picoseconds of the MD simulations to diffusion time scales, MC methods have been coupled to MD. During the workshop, different types of MC simulations were highlighted, namely the kinetic lattice MC, the kinetic object MC and the event MC. The kinetic and object MC describe the atom/vacancy thermal diffusion and the activated motion and reaction between extended clusters of defects respectively. The event MC is based on the calculated probability that two objects react within a certain time interval based upon the results of diffusion equations. Among the possible activated reactions, we may cite, as examples, vacancy emission from vacancy clusters, impurity/vacancy trapping and detrapping, SIA's cluster, vacancy cluster recombination etc. The main drawback of these methods is the large number of material parameters that need to be specified as input of the simulations. Those parameters can either be determined from MD and ab initio calculations or from experimental work. It remains that the overall parameterization of these models is an important issue for the validity of the results. It was suggested that careful parameter sensitivity studies should be run to increase the confidence in the predictions of the model. Using the MC techniques, the microstructural evolution in neutron-irradiated α-iron was investigated where the effect of temperature, of dose rate, of defect sinks such as GB and dislocations on the defect accumulation is discussed. Another study was presented where a kinetic MC model with input data from MD simulations was implemented that accounts for the microstructure evolution of fcc metals under irradiation in the presence of helium. In the latter case, the characteristic swelling curves of fcc metals as a function of temperature and dose rate was well reproduced.

2. Helium, other impurities and alloys stability

The production of gaseous impurities in structural materials of a fusion reactor remains an important issue that need to be further addressed. In the absence of a high energy fusion neutron source, that will reproduce the fusion He, H production and damage rates, this is one of the areas where modelling is expected to produce the necessary extrapolations from the available data from ion, fission and spallation source irradiation data. Depending on the irradiation temperature, He bubbles accumulate in the microstructures either at the GB or in the grain themselves and can cause severe embrittlement. It was recognized that the existing data are highly scattered, and is not easily comparable due to the numerous dissimilar irradiation conditions, and due to the different He production rate. In a near future, these inhomogeneities of helium generation and the control over the He/dpa ratio remain source of concern in this type of approach. Emerging techniques where He is produced by using a two-step thermal neutron reaction on ^{54}Fe and ^{55}Fe were mentioned. Depending on the reactor neutron spectrum, a He production rate up to about 2–4 appm/dpa can be expected. With this technique, the role of alloying elements (like B or Ni) in affecting the development of the irradiated microstructure will be avoided.

The mechanisms controlling the fate of He after its production in material of technological interest are not sufficiently known from the quantitative point of view. For instance, the transport of He along the GB or along the dislocations is still to be quantified. Further, binding energies of He with the defects of interest, trapping and detrapping energetics and resolution mechanisms are quantified only for few cases in pure material. These problems should be addressed using a combination of multiscale modelling and support experiments. For the time being, the additional hardening arising from a He bubble distribution is not well quantified. From punch tests experiment on tempered martensitic steels irradiated with a mixed spectrum of protons and neutrons in a spallation source at temperatures below 350 °C, it was shown that the He contribution to the embrittlement is likely to be a hardening one only for He contents above about 700–1000 appm. The observed hardening can be explained with contributions from the loop microstructure and a high density of nanovoids which have been detected by both positron annihilation and small angle neutron scattering after irradiations below 360 °C. The presence of helium though, does seem to increase the so-called ductile-to-brittle transition temperature beyond what is expected from the radiation hardening. Furthermore, for He content above 900 appm, there are indications that intergranular fracture starts to come into play. The conjugate effects of weakening the prior austenite grain and/or packet lath boundaries with He results in an increase of the DBTT shift. In another investigation, the effects of irradiation and helium implantation on the microstructural evolution, hardness and plastic deformation behaviour in Fe–15Cr–20Ni model austenitic ternary alloy and Fe–8∼9Cr–2W reduced activation martensitic steels were investigated through combined applications of ion irradiation, nano-indentation, focused ion-beam microprocessing and transmission electron microscopy. Systematic data on irradiation hardening were presented for various irradiation conditions. Influences of helium implantation on irradiation-induced microstructural and nano-indentation hardness changes were not clearly detected in the Fe–8∼9Cr–2W steels, while they were significant in the Fe–15Cr–20Ni alloy. Again, the various irradiation conditions indicate that the current information is not easily comparable due to the broad condition of irradiation conditions and material types.

Finally, MD and kinetic MC technique were also applied to study the growth and shrinkage mechanisms of helium-vacancy clusters in Fe. The dissociation energy of the clusters was calculated in function of the He density. These values of the dissociation energy were later used in a MC simulation, in which it was found that the He–V cluster is stabilized by the suppression of the thermal vacancy emission.

3. Defect–dislocation interactions, the evolution of the microstructure at large plastic strain and fracture

A new atomic model was presented that deals with the motion of an initially straight edge dislocation through voids and copper precipitates in α-iron. The mechanisms by which the dislocation overcomes the void or the copper precipitate were identified. It was shown that, in the case of copper precipitates, the interaction mechanism are dependent on the size of the precipitate, namely simple shear for precipitate diameters smaller than 2 nm and phase transformation towards a fcc structure of Cu for larger precipitates. It is worth emphasizing that this type of atomic-level simulation is essential to extract the necessary information used on a multiscale modelling approach.

A rather comprehensive review of the existing experimental observations on channelling was given. It is clear that flow localization is common in irradiated metals and alloys, where deformations channels are partly cleared of the irradiation induced defects. However, it was recognized that outstanding issues have to be resolved in order to build a comprehensive model of plasticity in which flow localization plays a role in the early stage of plastic deformation. We mention: (i) the effects SFT versus dislocation loops on defect cluster annihilation, (ii) the transmission of dislocation channels through GB, (iii) location of dislocation sources, (iv) stress and defect cluster spacing effects on flow localization, (v) effect of impurity segregation, (vi) role of the flow localization on the loss of ductility. A number of important issues were noted regarding the interaction between dislocations and irradiation-induced defects. Among these issues, there are: the strength of the obstacle, characterized by the coefficient α, the criterion for channel formation, the processes of channel clearing. Regarding the last point, it was recognized that the information obtained from the MD simulation involved large dislocation velocity due to the strain rates ($\sim 10^7$ s^{-1}) available from computer simulations, more than ten orders of magnitude larger than those at which the deformation experiments are normally performed. In addition, the role of cross-slip and stacking fault energy in defect clearing as well as the role of gas bubble against voids and that of local heating remains open issues.

The interaction problem of gliding dislocations with immobile dislocation loops and defects such as SFT's was studied analytically and computationally based on both statistical analysis and on a recently developed model of discrete stochastic dislocation dynamics (SDD). The SDD accounts for thermal activation mechanisms of metastable pinned dislocations using a stochastic force and for the motion process between metastable dislocation configurations under drag mechanisms.

Two reviews devoted to fracture where presented. One was a short examination of the experimental observations and the theoretical understanding of the fracture behaviour of tungsten in the brittle and semi-brittle regime. These experiments were carried out on tungsten single crystal. Dislocation simulations were used to analyze the dependence of the intrinsic fracture toughness on pre-deformation, temperature or loading rate in the transition regime. It was shown that dislocation nucleation is the limiting factor at low temperatures, while the dependence on loading rate at intermediate temperatures requires that dislocation mobility takes control. It was pointed out that the understanding of slightly more complicated microstructures and particularly of pre-deformed single crystals and/or textured and possibly pre-deformed polycrystalline materials is far less well understood and that more experiments are needed to investigate the role of dislocations, microcracking, branching of the main crack and crack bridging effects. The second presentation outlined the role of fracture mechanics and the importance of irradiation embrittlement in the design and operation of fusion first wall and blanket structures, based on the master-curve method. Similarly to the evolution of the irradiated microstructure that has to be investigated on a multiscale approach, the sequence of processes that control fracture start on the atomic scale and proceed to meso and macroscopic scales. The possibility of using the master-curve concept for the tempered martensitic steel was thoroughly discussed in this context. Furthermore, a possible explanation for the constant shape the master curve was proposed, explanation that lies in the intrinsic characteristics of the bcc ferrite lattice.