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Editors' summary

Basic aspects of differences in irradiation effects between fcc, bcc and hcp metals and alloys

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The present workshop dealt with the fundamental aspects of the effect of crystal structure on defect production and accumulation in metallic materials. The papers included in these proceedings are review papers providing an update of the state of art in the field of irradiation damage in metals as well as original contributions to clarify these aspects from different points of view.

Due to the very tight time schedule, it was not possible however for the Review Committee, which was in charge to prepare a Summary as it was the tradition in previous workshops of these series, to discuss thoroughly all the presentations. Therefore, the organisers as editors have taken the responsibility of outlining the most salient issues discussed during the workshop.

The workshop addressed the similarities and differences in damage production arising from variances in the crystal structure. A basic difference can be expected in the behaviour of the isotropic fcc and bcc structures as compared to the anisotropic hcp one, but further differences could be expected between the compact fcc configuration and the more open bcc structure. Starting from these elementary considerations, the workshop considered how they affected the displacement cascade evolution and defect accumulation.

In terms of computer simulation of the cascade event and microstructure evolution, progress has been made in investigating the cascade damage from single events to multicascade effects, and in the assessment of other effects such the presence of a surface in the vicinity of the cascade zone, and the matrix temperature. The main difference between fcc and bcc metals lies in the defect cluster size distribution after the cooling down phase of the cascades. In fact, molecular dynamic (MD) simulations have revealed that for the same recoil energy, both the fraction and the size of self-interstitial atom (SIA) clusters present at the end of the collision cascade are larger in Cu than in Fe.

By combining MD with Monte Carlo (MC) methods, the time scale of simulations can be extended from picoseconds to observable times. However, the workshop highlighted the need for the acquisition of reliable input parameters (i.e., choice of potential, intrinsic defect properties, etc.) in order to obtain meaningful simulation results. Effort is already in progress to determine these parameters, both in ongoing experiments and simulation calculations. These parameters are vital for the quality and the reliability of results that can be obtained from the combination of MD and MC.

Further differences between fcc and bcc pure metals have been investigated using hierarchical simulation methods. It was made clear by all participants that this kind of computer simulation has to address the questions of the stability, mobility and interaction of defects that are produced in the cascades. In this sense, probably the most significant issue discussed is the 1D-migration mechanism of SIA clusters, to which several contributions are devoted. The results of the simulation highlighted two important aspects of the behaviour of SIA clusters. First, it was demonstrated that the one-dimensionally diffusing SIA clusters change their Burger's vector (i.e., direction of diffusion) during their life time both in fcc and bcc metals. However, there was not enough results to quantify the frequency of such changes. The second significant observation refers to the fraction of glissile SIA clusters produced in the cascades. The results reported gave a clear indication that this

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fraction is likely to be substantially higher in bcc than that in fcc metals. Furthermore, relaxation MD simulations were reported to show that even those SIA clusters that may be produced with a sessile configuration in Fe, may very quickly transform themselves into a glissile configuration. In fact, depending on the relative orientation of the Burger's vector of two neighbouring clusters, they might attract each other (growth), or become immobile (pinning).

Some of the simulation results on the cascade characteristics and defect accumulation are already being included in the more realistic analytical modelling of the microstructure evolution which was presented. The recognition of the fact that the defect produced in displacement cascades are not homogeneously distributed has previously led to the concept of production bias, which includes the effect of glissile clusters and the consideration of size distribution functions. The work presented at the workshop included the treatment of changes in Burger's vector of the one-dimensionally diffusing SIA clusters. These refinements make the prediction of the defect accumulation kinetics more quantitative. The discussion indicated that the model is applicable in their present state to pure metals and needs further development to be extended to technological materials.

Two new important topics dealing with the origin of radiation hardening were analysed. First, results on the elastic interaction of a dislocation with glissile defect clusters were presented, showing that the clusters are likely to be trapped by an edge dislocation at distances of about 10 nm in bcc and 20 nm in the fcc structure and that both in bcc Fe and fcc Cu, clusters near the core of the dislocation can be absorbed after a rotation of their Burger's vector induced by the elastic force field. These simulations, which are at the base of our understanding of the mechanical behaviour of the irradiated metal, will have to be performed as atomistic calculations. The second topic is that of the simulation of stress–strain behaviour with 3D dislocation dynamics, which provides a natural transition from the atomic to the continuum crystal scale. Here again, the initial treatment of the case of loops decorating the dislocations indicates clearly that the future lies in a linkage of this type of simulation to MD calculations of the details of the dislocation defect cluster interaction.

Regarding the experimental database on fundamental differences between fcc, bcc and hcp metals and alloys, the presentations on this subject made it clear that because of the present lack of well designed experiments, especially in hcp metals and alloys, no convincing conclusions can be drawn regarding the complete set of crystal structures. But clear differences have been found between fcc and bcc in the defect accumulation behaviour: nearly three orders of magnitude higher dose is needed to attain the same cluster density in bcc Fe than that in fcc Cu. There are also clear indications that the stacking fault energy plays a role in determining the type of preponderant defect cluster observed. Another significant difference was, for the first time demonstrated experimentally, that the neutron irradiation at 100°C causes void formation in bcc Fe but not in fcc Cu.

Differences in the swelling behaviour between austenitic and ferritic steels were reviewed and it is argued that the main difference arises from the longer transient regimes in the bcc steels, while the corresponding steady state swelling is around 0.2% per dpa as compared to 1% per dpa in the austenitics.

In terms of deformation, in both bcc and fcc structures it was shown that the main deformation mode is dislocation channeling, with deformation twinning as an alternative mechanism in stainless steels. In both cases, it leads to extremely localised deformation at grain boundary microcracking. This has lead to the idea of analysing the data in terms of deformation maps as a useful manner of displaying the relations of deformation and fracture mechanisms to defect microstructure and parameters such as strain rate and temperature.