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The influence of Helium bubbles on the critical resolved shear stress of dispersion strengthened alloys

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ABSTRACT

Dispersoid strengthening is particularly important for ferritic based structural components used in nuclear applications due to their superior radiation resistance and creep strength at high temperatures. Within nuclear technologies yttrium particles dispersed throughout the matrix are the most promising ferritic steels to achieve these improved materials properties by acting as obstacles to dislocation motion. Due to radiation damage in these alloys considerable production of helium bubbles can be observed. Their amalgamation into large structures can be detrimental to the material's lifetime and it is therefore important to understand how their interaction with other defects can be controlled and what effect their presence has. Increased computational power now allows the direct study of such dislocation-obstacle interactions using 3D Discrete Dislocation Dynamics simulations at the mesoscale. In this work the effect of helium bubbles in irradiated dispersion strengthened ferritic steels and the response of the critical resolved shear stress is studied and found to increase with the density of helium bubbles.

1. Introduction

There is a growing focus on ferritic steels as candidate structural materials for future fusion reactor walls. Fusion reactors will experience considerable production of Helium (He) by (n,α) reactions (10 and 150 appm/dpa, respectively) due to radiation damage processes. The atoms can easily precipitate into bubbles due to very low insolubility, resulting in a large increase in yield stress at lower irradiation temperatures. In time, these bubbles coalesce and lead to fatigue and fracture of the material. In fission reactors, the interaction between He and microstructural defects, which determines the mechanical properties of the structural materials, is currently not well understood [1,2] and high dpa rate experiments performed to date under-predict swelling in reactors operating at lower flux (such as will be the case in the VHTR) indicating that He's role in future fission reactors may be underestimated by experiments done today. Indeed, the presence and effect of He is of concern over a wide range of temperatures [3–5] relevant to both fission and fusion environments. He can cluster to intragranular voids or it can diffuse to grain boundaries to form voids there. Voids at grain boundaries should be avoided under creep loading conditions which also promotes void formation. It is therefore advantageous to keep the helium in the matrix. Very fine dispersoids in ODS alloys can for example act as sinks for helium. Larger dispersoids present in conventional ODS alloys are not as effective and microstructures consisting of bubbles and dispersoids can develop. Therefore it is important to understand the contribution of intragranular helium bubbles to the strength and other mechanical properties of the material in question.

Because experimental investigation of material's response in simulated experimental environments is difficult and lengthy, multiscale modelling studies investigating changes in materials mechanical properties under irradiation, high temperatures, or corrosive environment are becoming a complementary method expected to speed up and enhance the understanding of materials' mechanical properties in extreme environments. Atomistic simulations have shown that interstitial helium with low migration energy and substitutional helium which has a large trapping energy are the two main configurations identified to contribute to helium accumulation [6]. However, as atomistic simulations cannot deal with large samples and time scales and focus only on interactions of dislocations with one or two lattice defects, mesoscale Discrete Dislocation Dynamics (DDD) simulations prove to be very useful tool to study the mechanical properties of particle enforced alloys, enabling the study of longer time and length scales as well as more realistic stress and strain rates than what is possible in MD simulations.

To understand the influence of helium bubbles in ferritic steels, in this paper we undertake the study of how helium affects ODS ferritic steels, where the main factor in determining the CRSS of as dislocations traversing the material has been found to be the

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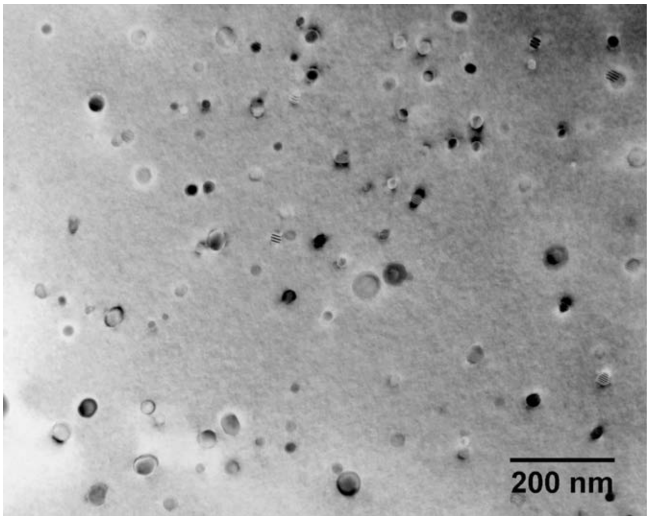

Fig. 1. Typical TEM image of PM2000 illustrating the Y_2O_3 dispersoids

presence of the ODS particles [7]. Mesoscale DDD simulations were performed on samples generated using a quantitative determination of the contribution of Y_2O_3 dispersoids and He bubbles to the strength of PM2000, a high-resistant Fe-Cr-Al commercial alloy with nominal chemical composition in weight%: 19 Cr / 5.5 Al / 0.5 Ti / 0.5 Y_2O_3 / remainder Fe [8].

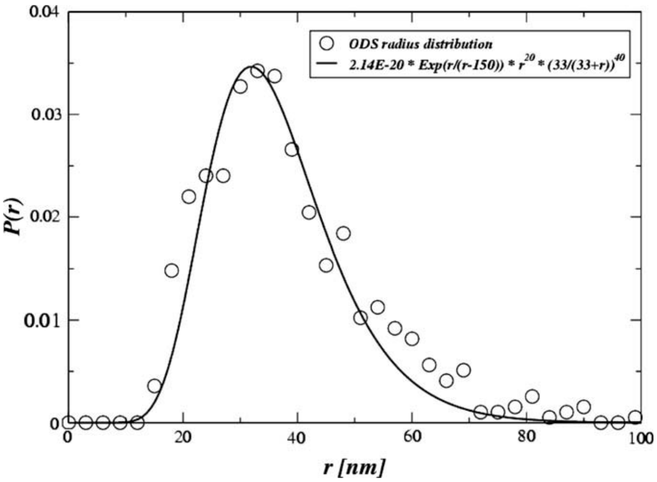

Fig. 2. ODS particle radius probability distribution function.

2. The model

The DDD simulations are based on the continuum description of dislocations, discretized using connected straight segments, whose line direction can vary continuously between pure screw and pure edge orientation. The model relies on physical assumptions, so called constitutive rules for the equation of motion. A linear relation between the driving force, the resolved Peach-Koehler force, and the velocity is assumed and the evolution of the nodal positions is obtained by simple Euler forward integration scheme [9]. The drag coefficient of the dislocations is assumed to depend on the character of the dislocation as

$$M(\phi) = M_s \cos^2(\phi) + M_e \sin^2(\phi),$$

where M_s and M_e are the drag coefficient of pure screw and edge dislocation segments, respectively. The angle φ is defined as the angle between the Burgers vector and line direction vector of the segments. Further details on the DDD model can be found in [9].

To obtain more realistic results in the simulations, the size distribution of the ODS particles is measured experimentally by means of TEM and this distribution is used in the DDD model. The analysis is based on several TEM micrographs, taken from thin specimens of the ferritic steel PM2000 with a thickness of approximately 200 nm, which has been used in previous DDD studies to understand the effect of particle hardening on the mechanical properties [7]. In this paper, the additional effect of including helium is addressed. The sample preparation method is described in details in [10] and [11]. A typical PM2000 TEM image used in the particle diameter analysis is presented in Fig. 1.

To determine the size distribution, an automated particle analysis [7] was performed using the program **ImageJ** [12]. After background removal, the particles were defined by a threshold grey level of digitized TEM images. For a more precise radius determination of the spherical ODS particles, the particles were assumed to have an elliptic shape during the image processing. The average value of the minor and major axis distributions of the particles from the TEM images is shown in Fig. 2. The volume fraction of Y_2O_3 dispersoids was determined to be approximatively 0.6%, with an average diameter of 28 nm and number density 5.1×10^{20} particles/m^3 [13].

The data used as input for the He bubble formation is taken from studies in AISI 304L a commercial austenitic stainless steel (with nominal chemical composition in wt.% 10.0/12.5 Ni, 17.0/20.0 Cr, 0.03 S, 0.045 P, $\leqslant$2.0 Mn, $\leqslant$1.0 Si, and $\leqslant$0.03 C), a candidate for structural materials in future high-power spallation neutron sources. The sample was irradiated with 800 MeV protons and annealed at 810 °C. A typical micrograph and the He bubble size distributions are given in Fig. 3 a) and b) respectively. It was found

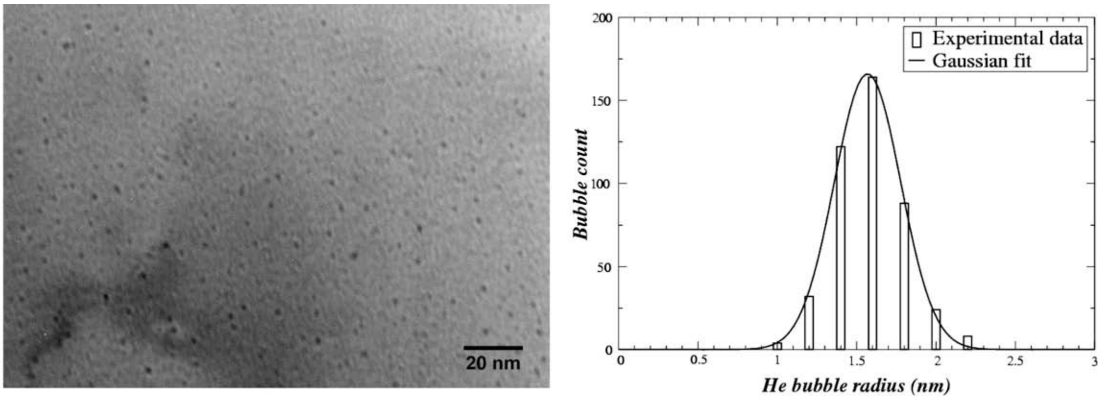

Fig. 3. Typical AISI 304L TEM image with He bubbles (left) and their size distribution (right).

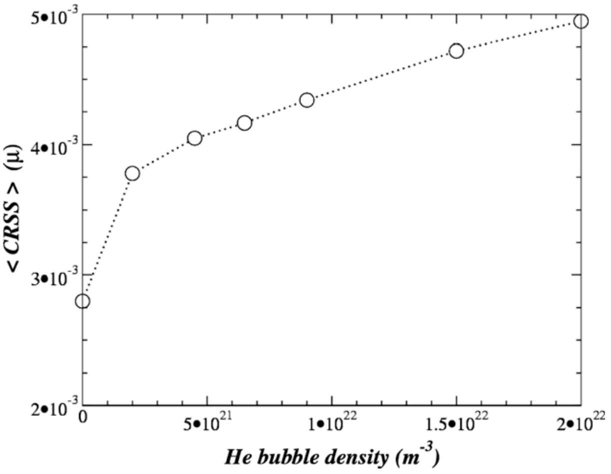

Fig. 4. CRSS of PM2000 alloy as function of the Helium bubble density.

that the mean bubble diameter is 1.48 nm and the bubble density 2.0×10^{23} m^{-3} [12]. These parameters for the bubble and ODS size and distribution have then been implemented into the model.

3. Simulation setup and results

For technical applications it is important to know how the changes in obstacle (i.e. He bubble) size and density affect the flow stress of materials. The change in the CRSS, defined as the change in the resolved shear stress necessary for dislocations to glide freely, gives an indication of how the material's properties are modified as more and more He bubbles are created by radiation in the matrix.

To study the change in the CRSS caused by the He bubbles, 25 random ODS distributions were generated. The spatial arrangement of particles was considered to be a random variable in 3D, with uniform distribution, and the constraint that no particles overlap [14]. The radius of ODS particles was also randomly chosen from the probability distribution function of ODS particles experimentally determined for PM2000, shown in Fig. 2. Spherical He bubbles were generated with uniform distribution in space. Their random radii were picked from a Gaussian distribution with mean 1.5 nm and half width 0.5 nm. The density of He bubbles studied was in the 0 to 2.0×10^{23} m^{-3} range.

An initially straight screw dislocation with line direction parallel to the (1 -1 1) direction was created on the (1 1 0) slip plane containing the centre of the 1 μm cubic simulation cell. Periodic boundary conditions in the (1 -1 1) direction make the dislocation line infinitely long. The resolved shear stress resulting from an applied stress on the dislocation drives the motion of the dislocation through the obstacle field. Based on MD simulations, He bubbles are strong obstacles [15]. In our simulations ODS particles and the He bubbles were considered hard core spheres, which is a reasonable approximation [7,14]. The materials parameters for the BCC Fe matrix used in the simulations were: shear modulus μ = 86 GPa, Poisson ratio υ = 0.291, lattice constant a = 0.287 nm, Peierls stress $\tau_p = 10^{-3}\ \mu$. The drag coefficients were taken as the values for iron single crystals at room temperature measured by Urabe and Weertman [16]: 0.66 Pa s for screw, and 0.345 Pa s for edge character dislocation segments.

The CRSS was obtained as the average of 25 random, statistically equivalent arrangements of ODS particles and He bubbles. The density of He bubbles was increased up to the value of 2.0×10^{22} m^{-3}. The increase of the bubble density causes a dramatic increase of the CRSS, with a factor of 2 relative to the non-irradiated samples (see Fig. 4). This is in agreement with the experimental results [1] where an additional hardening/embrittlement is observed for helium contents of around 1 at.% and larger. Time and money constraints of undertaking experiments on the same order as the results produced in these DDD simulations emphasis the advantage of using such modelling techniques to understand the hardening/embrittlement of materials under irradiation.

4. Conclusions

The critical resolved shear stress of irradiated PM2000, a dispersion strengthened ferritic steel was studied by computer simulations. The experimentally determined oxide dispersoid size distribution of PM2000 was used as input for the numerical model. The simulations with randomly distributed dispersoids and He bubbles show that the critical stress increases with the increase of the radiation induced bubble density and emphasize the importance of integrating modelling into materials research to obtain a deeper understanding of the material's behavior.

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