Theoretical and Experimental Investigation on Nanoparticles within 14YWT

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Biography

Current PhD focusing on both numerical and experimental characterization of novel materials. Experience with density functional theory (DFT) simulation and synchrotron X-ray diffraction (XRD) technique. Received Bachelor of Science degree in Huazhong University of Science and Technology, Wuhan, China.

Overview:

14YWT is a type of nanostructured ferritic alloy which exhibits excellent mechanical strength and irradiation resistance under harsh nuclear reaction conditions. Such exceptional properties are attributed to the 2-4nm Y-Ti-O enriched nanoclusters (NCs) dispersed in ultrahigh density within the ferritic matrix. These NCs act as effect pins to dislocation slipping and grain boundary gliding during deformation. At the same time, NCs can trap irradiation induced helium bubbles into small size (1-2nm) and uniform distribution, thus enhancing the irradiation resistance. This work aims to elucidate the mechanism of NCs to limit helium bubble size with DFT calculation and the role of NCs in improving the mechanical strength of 14YWT with synchrotron XRD experiment.

Motivation

With the increasing demand in energy consumption and electricity generation, nuclear systems with high efficiency and security are proposed. The structural components in the system have to withstand harsh nuclear reaction conditions and structural materials with excellent properties are required. 14YWT is a promising candidate for the structural material in nuclear reactors. It is reported to maintain mechanical integrity under high temperature, high pressure and high irradiation conditions. However, the mechanism of its high resistance to elevated temperature and irradiation induced damage is not clear. It is of great importance to understand the underlying reasons for such excellent material properties, which will largely benefit future design of structural materials in nuclear industry.

State of the Art

Fu et. al. have demonstrated with DFT calculation that the prerequisite for the formation of NCs is oxygen: vacancy pairs (O:Vac pair). [1] Zhao et. al. further proved that the O:Vac pairs can attract solute atoms Ti and Y, and eventually develop into 2-4nm NCs with exceptionally stable interface. [2] Researchers have been first seeking the understanding of the formation and growth criteria of He bubbles within BCC-Fe matrix under irradiation. From DFT calculations, researchers found that He atoms have tendency to occupy the tetrahedral interstitial positions in iron matrix. [3] He atoms can form strong binding with pre-existing vacancies and the stability of small He-vacancy clusters has been investigated. [4] However, the helium bubble behavior near NCs are not tackled. The theoretical study of NCs influence on the mechanical performance of NFAs is very limited. Extensive experimental works has been conducted to show that despite the contribution from grain and dislocation structures, NCs contribute greatly to the enhancement in tensile and creep strength of NFAs via load partitioning mechanism. [5] The NCs hardening are predicted to be 400MPa in MA957 and 12YWT from the dispersed-barrier-hardening model. [6] However, the strengthening mechanism of NCs in 14YWT, especially at high temperatures, is not addressed.

Intellectual Merit

This work mainly tackles,

1. NCs' role in limiting helium bubble size and in enhancing irradiation damages
2. NCs' role in strengthening in 14YWT, especially at elevated temperatures

The first hypothesis is that NCs in 14YWT can effectively trap the irradiation generated helium atoms, at the same time impose constrain on the growing of helium bubbles, such that the helium bubbles are limited to small size and ultra-high density as the NCs. The second hypothesis is that NCs can share certain part of external loading from the ferritic matrix and thus enhance the mechanical strength of 14YWT during deformation. If completed, this work not only serves as a handbook for the application of 14YWT, but also provides guidance for future design of new-type NFAs with higher strength and irradiation resistance.

Broader Impact

Firstly, it can provide the detailed properties of 14YWT in its future application. Secondly, it shows the mechanisms of how NCs improve the mechanical strength and irradiation resistance in 14YWT, which is of great significance to the future design of NCs size and composition in new generation NFAs. With the further increase in the excellency of the structural material, nuclear systems can escalate with higher efficiency and security.

Research Approach

1. Numerical simulation

   DFT calculation is adopted to study the helium behavior near NCs in 14YWT and elucidate NCs' role in limiting the helium bubble size and enhancing the irradiation resistance. Nano-scale modeling is feasible with DFT calculation and does not suffer from inaccuracy in interatomic potential as other simulation methods (Molecular dynamics, Monte Carlo method) may do. But the simulation of actual size 2-4nm NC and 1-2nm helium bubble is implausible due to computation limit. Thus a smaller domain of ferritic matrix embedded with typical NC unit cell will be considered. The interaction between NCs and helium bubbles will be analyzed by energetic study.

2. Experimental testing

   In-situ synchrotron XRD technique will be used during uniaxial tensile test in 14YWT at room temperature (RT), 300°C, 500°C and 600°C. Another previously developed type of NFA, which is labeled 9YWTV, will be tested under the same conditions for comparison. It is hard to directly observe the strengthening effect of NCs in 14YWT due to its small size and nonstoichiometric nature. Thus the strengthening effect of NCs will be studied by comparing mean internal stress and actual applied stress from *in-situ* synchrotron XRD experiment.

Findings to Date

1. NCs' role in limiting helium bubble size and enhancing irradiation damages

   NCs can trap helium atoms with O:Vac pairs. In addition O:Vac, Ti and Y can reduce the stable helium bubble size. Thus the helium bubbles can be of similar density of NCs and maintain a small size. Without the presence of large helium bubbles, the resistance to irradiation is enhanced.

2. NCs' role in strengthening in 14YWT, especially at elevated temperatures

   The applied stress is higher than mean internal stress in 14YWT at all temperatures, indicating the load transfer from the ferritic matrix to NCs in 4YWT, thus the mechanical strength is enhanced. Meanwhile, the applied stress is almost the same as mean internal stress in 9YWTV at higher temperatures, denoting the NCs strengthening effect in 14YWT is stronger than that in 9YWTV.

Conclusions

1. NCs in 14YWT can effectively trap helium and reduce the helium bubble size, thus leading to the enhancement in irradiation resistance.

2. NCs can strengthen 14YWT with load transfer mechanism both at room temperature and elevated temperatures.

References

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