8.3 DEVELOPMENT OF A NEW EQUATION OF STATE FOR HELIUM IN IRON —

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OBJECTIVE

The objective of this research is to develop the modeling and simulation tools necessary to improve our understanding of how helium interacts with other defects in iron-based alloys to produce changes in the microstructure and mechanical properties.

SUMMARY

A large series of molecular dynamics simulations are underway to provide the detailed atomistic data, which will enable final fitting of a new equation of state for helium in iron. This potential will be based on the behavior of helium as described by the three-body Fe-He potential developed at ORNL under the fusion program.

PROGRESS AND STATUS

Introduction

Because of the high helium levels generated by nuclear transmutation reactions, predictions of structural material performance under DT fusion conditions must account for how the helium influences microstructural evolution and the related mechanical properties. One of the primary issues that must be addressed is the behavior of He-vacancy clusters, which evolve, into finite-sized bubbles with the potential for growing into voids. In this case, a 'bubble' is defined as a cavity, which is stabilized by the helium pressure it contains. If helium is removed a bubble will shrink. In contrast, a 'void' is a cavity, which has grown large enough that growth can be maintained by the absorption of a net vacancy flux. The gas pressure plays essentially no role in voids stability. The properties of small He-vacancy clusters, such as the helium and vacancy binding energy are critical to predicting bubble stability. These processes can only be accurately described by atomistic simulations such as molecular dynamics (MD), which requires an interatomic potential to describe the behavior of both the metal and helium atoms. In order to improve our predictive capability for the Fe-based materials of most interest to fusion structural applications, a new Fe-He interatomic potential was developed based on ab initio calculations of the interactions between He and point defects in Fe [1-2]. Additional work using this potential as characterized the properties of small He-vacancy clusters and parameters such as the He-to-vacancy ratio as a function if cluster/bubble size and temperature [3-4]. The observations of that work is being extended to develop an atomistic equation of state for helium in iron which can then be applied in a broad range of mesoscale to predict microstructural evolution.

Current Progress

In order to provide a basis for fitting the pressure-temperature relationship required for the equation of state (EOS), a series of MD simulations has been initiated. The primary conditions are described in Table 1. The temperature range was chosen to cover a range, which includes much lower and higher temperatures than the expected applications of the EOS. The bubble sizes encompass those of interest to fusion reactor materials, and an accurate extrapolation to larger sizes will be verified. If needed, larger sizes may be included, although the expectation

is that the pressure will be sufficiently low at large sizes that a more simple equation of state will be appropriate. For each of the bubble sizes, the pressure will be obtained for a broad range of He/vacancy ratios, from highly over-pressurized to a void-like under-pressurized state. The pressure at mechanical equilibrium will also be determined.

The primary issue in fitting the EOS is to choose an appropriate function to describe the compressibility of the gas. We will first adopt the hard-sphere model of Brearley and MacInnes [5] for testing and evaluation. One difference between the atomistic results and the assumptions typically applied in developing an EOS is illustrated in Fig. 1. The general thought is that the gas atoms occupy the complete bubble volume. However, MD simulations using the ORNL Fe-He potential in concert with the Fe potential of Ackland, et al. [6] indicate that the Fe-He interaction leads to a small exclusion volume near the bubble surface. This is demonstrated in Fig. 1a in which the time-averaged positions of the iron surface atoms (green) and helium atoms (gold) are shown. Fig. 1b shows the corresponding radial distribution of He atoms graphically. The result of this standoff distance is that the effective volume of the bubble used to compute the pressure is smaller and the pressure is higher.

Table 1. Conditions for MD simulations

Temperature (K)	Bubble radius (nm)
200	0.25, 0.5, 1.0, 2.0, 5.0
300	same as above
400	same as above
500	same as above
600	same as above
700	same as above
800	same as above
900	same as above
1000	same as above
1100	same as above

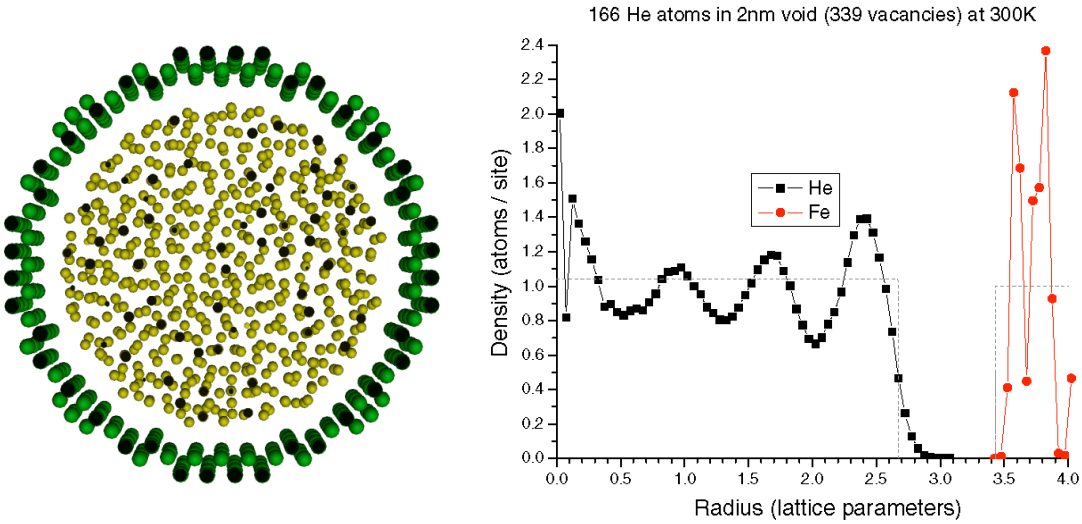

Fig. 1. Illustration of how Fe-He interaction leads to the formation of a gas-free region near the bubble surface for a 2 nm diameter bubble [4].

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