**HARDENING DUE TO HE-FILLED BUBBLES IN IRON –** Yu. N. Osetskiy, R. E. Stoller and D. Stewart (Oak Ridge National Laboratory)

## OBJECTIVE

This work has as an objective to understand the state of He-filled bubbles in Fe and their effect on the mechanical properties of irradiated Fe.

## SUMMARY

Gas-filled bubble strengthening is an important radiation effect observed in structural materials subjected to high dose irradiation at moderate temperature. The usual treatment of this effect is based on the continuum approach to estimate the equilibrium state of gas bubbles and simplified estimation of their strengthening on the basis of line tension models. We suggest employing multi-scale computer modeling to investigate such effects. This includes low level Density Functional Theory (DFT) calculations to construct an empirical potential for interatomic interactions in Metal-Gas system. Such calculations need up to a few hundred atoms and their free electrons. Next level includes Molecular Dynamics (MD) technique to investigate the equilibrium state of gas filled bubbles as a function of their size and ambient temperature. The scale covered at this level includes bubble of size up to 10nm in matrix crystals of up to 2-4x$10^6$ atoms. Finally, MD modeling of interactions between moving dislocations and gas-filled bubbles is the largest scale in this approach considering up to $10^8$ atoms modeled over a few nanosecond simulated time. This cutting edge research has started at ORNL and will demand significant computational and intellectual resources over the next few next years. We present here the first few results of a multi-scale study of He-bubbles in Fe obtained during FY 2009.

## PROGRESS AND STATUS

### Atomic-scale model

To study Fe-He system at atomic scale a set of three interatomic potentials (IAPs) is necessary to describe interactions between matrix atoms (Fe-Fe), between He atoms inside bubbles (He-He) and also Fe-He interactions. The Fe-He potential recently developed at ORNL within the Fusion Materials Program was employed here [1, 2]. This potential describes three-body interactions between Fe and He atoms and was fitted to DFT data on forces and energies of different defect including He-vacancy clusters. In the present research IAPs for He-He and Fe-Fe are taken from refs. [3] and [4] respectively.

The above IAPs are used in molecular dynamics (MD) and statics (MS) modeling of He-filled bubbles in Fe. Surface energy of voids was estimated by modeling voids at zero temperature by MS. Crystals of up to 2x$10^6$ atoms were relaxed by a combination of conjugant gradients + quasi-dynamics. Equilibrium state of bubbles at different temperatures was studied by MD modeling at constant temperature over the range from 100 to 900 K over time of 300 ps. Interactions between moving edge dislocation ½<111>{110} and 2 nm bubbles at different temperature and He was simulated using a modification of the model described in [5]. Dislocations were moved under applied strain with rate $10^7$ $s^{-1}$. Such simulations allow obtaining stress-strain information, maximum stress necessary to overcome an obstacle and dislocation line shape at any applied stress.

### Surface energy.

Surface energy $\gamma$ is necessary to estimate a pressure $P$ inside a bubble of radius $R$ using the capillarity model : $P=2\gamma/R$, used so far in theoretical predictions. We have estimated surface energy through void formation energy $E_V$ as : $E_V = 3/4\pi R^2\gamma$.

In Fig.1 we present the dependence of the void formation energy and the corresponding surface energy estimated for voids of radius up to 10 nm. It can seen that void surface energy depends on radius for small voids but saturates at a value ~1.82 J/$m^2$ for voids larger than $R \approx 5$ nm.

Values of void surface energy obtained in static modeling were used for estimation of pressure inside bubbles in terms of the capillarity model and the results are presented in Fig.2.

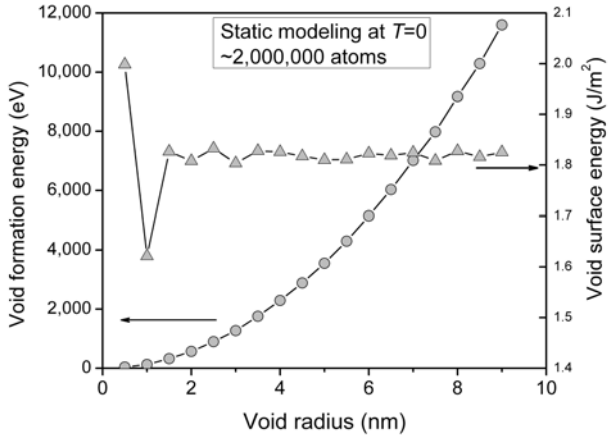


Fig.1 Void formation energy (circles) and the corresponding void surface energy (triangles) estimated for voids of different size.

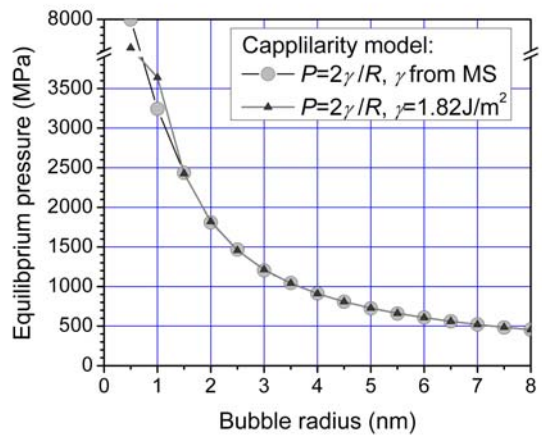


Fig.2 Equilibrium pressure for bubbles of different size using capillarity model and data from static modeling of voids.

The capillarity model usually used for such estimations have a number of deficiencies such as neglect of the bubble temperature and properties of matrix material. We therefore have applied MD to estimate equilibrium pressure as function of the ambient temperature and bubble radius. The criterion of equilibrium adopted here is a zero total dilatation of the bubble at different conditions. In practice we simulated bubble at the desired temperature and varied the number of He atoms inside until the total pressure in the simulated system is zero after annealing for 300 ps. The results are presented in Fig.3 and are compared with the values estimated above using capillarity model.

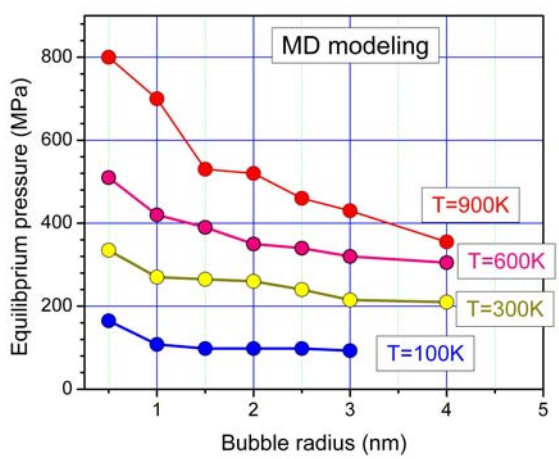


Fig.3 Equilibrium pressure of He inside bubbles of different size at different temperatures.

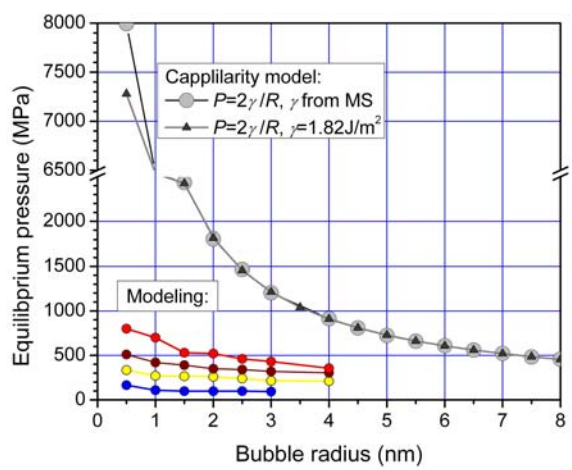


Fig.4 Comparison of bubble pressure estimated within capillarity model (grey circles and triangles) and equilibrium pressure of He estimated in MD modeling.

A comparison shows that the value of pressure estimated in MD modeling is significantly lower than that from capillarity model and the difference increases for small bubbles and low temperature.

This difference will be evaluated in future studies.

**Bubble hardening.**

Hardening effects due to bubbles was investigated by MD for the example of interaction with edge dislocation with ½<111> Burgers vector gliding on {110} plane. A bubble of 2 nm radius with its equator on the dislocation slip plane was placed 10 nm from the core in the direction of its motion. In this report we present first results with a relatively fast dislocation moving at 28 m/s under applied strain rate $10^7$ $s^{-1}$. Lower applied strain rates are in progress as well as bubbles of radii 1 and 4 nm.

Maximum stress at which dislocations bypass the bubble at different temperatures and He/Vacancy content is presented in Fig.5. The results are compared with void of the same size simulated earlier.

Several qualitatively new results are obtained in this initial research. Thus, bubble with He/Vac = 0.5, that corresponds to close to equilibrium pressure in the above MD study, demonstrate the maximum hardening effect. Slightly under- and over- pressurized bubbles with He/Vac = 0.25 and 0.75 are softer than the equilibrium bubble, however, they are compatible or stronger than a void. The mechanism for the dislocation bypass of bubbles with He/Vac ≤ 1 is the same as for voids – the dislocation cuts and shears bubbles in the same way as void. However, at He/Vac = 2 we have observed that a relatively large glissile dislocation loops is emitted from the bubble when the dislocation approaches it. This loop then is absorbed by the dislocation as a superjog. In this mechanism the dislocation does not cut the bubble and the bubble size is increased after interaction. Temperature dependence of this interaction is opposite to that for lower He/Vac content.

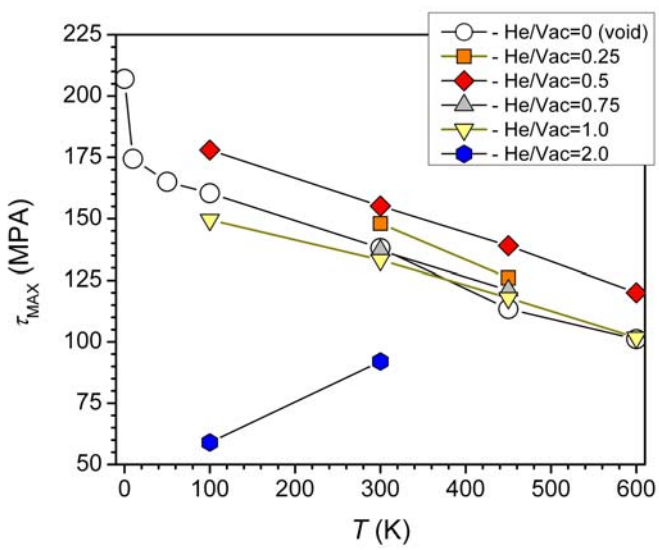


Fig.5 Critical resolved shear stress for edge dislocation ½<111>{110} to overcome a row of 2nm bubbles with different He content (He/Vac ratio) at different ambient temperature.

**FUTURE STUDIES**

1. Investigation of the equation of state for He-filled bubbles as function of bubble size, matrix properties and ambient temperature.
2. Understanding of the interaction mechanism, especially for equilibrium bubbles.
3. Simulation of bubbles of other sizes with another equilibrium He/Vac ratios.
4. Screw and mixed dislocations will be simulated.
5. Strain rate (dislocation velocity) effect will be investigated.

## References


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