8.4 A STOCHASTIC NONLINEAR DIFFERENTIAL EQUATIONS APPROACH TO THE SOLUTION OF THE HELIUM BUBBLE SIZE DISTRIBUTION IN IRRADIATED METALS- D. Seif (University of California, Los Angeles), N.M. Ghoniem (University of California, Los Angeles)

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A rate theory model based on the theory of nonlinear stochastic differential equations (SDEs) is developed to estimate the time-dependent size distribution of helium bubbles in metals under irradiation. Using approaches derived from Ito's calculus [1], rate equations for the first five moments of the size distribution in helium-vacancy space are derived, accounting for the stochastic nature of the atomic processes involved. Fluctuations and the spread of the distribution about the mean are obtained by white-noise terms in the second-order moments. Physically, these are driven by fluctuations in the general absorption and emission of point defects by bubbles and fluctuations stemming from collision cascades. This statistical model for the reconstruction of the distribution by its moments is coupled to a previously developed reduced-set rate theory model [2], which has been shown to adequately describe the nucleation and growth phases of average-sized bubbles in irradiated metals.

As an illustrative case study, the model is applied to a tungsten plasma-facing component under irradiation, at a dose rate of $5X10^{-3}$ dpa/s and with a He/dpa ratio of 5 appm/dpa. The results of a simulation at 1800 K are shown in figure 1, showing the evolution of the distribution in the first 200 seconds of irradiation time. Projections of the vacancy and helium profiles of the distribution are seen in blue and red, respectively, and the mean bubble radius and mean pressure ratio, P/P_{eq}, are plotted in the inset plot on the left and right ordinate axes, respectively. In the very early stages of irradiation, we observe a rapid spreading of the distribution in the vacancy direction, which continues to grow, stabilizing after about 100 seconds of irradiation. This rapid dispersion stems from the increased effect of the stochastic fluctuations when bubble sizes are very small. The stabilization begins to occur as the average bubble size increases. In these early times, from the nucleation regime until the average bubble reaches roughly 3 nm, bubbles are observed to be highly pressurized (P/P_{eq}>>1). Due to the large difference in mobilities, when bubble concentrations and sizes are small, helium atoms can more effectively find their way to bubbles leading to these large pressures. However, as the internal helium interstitial population decreases due to bubble capture, the vacancy capture rates become large enough to keep the pressures low. The steady state bubble pressures are strongly controlled by the helium generation rate, H, and the re-solution parameter, b, which can be tuned to replicate specific experimental data. Figure 2 shows the time evolution during the simulation of the moments of the distribution (m_{10}, m_{01}, m_{20}, m_{02}, and m_{11}, where m_{ij} is the ith moment in the helium direction and j^{th} moment in the vacancy direction).

The primary advantage of the method is the necessity for only a small set of rate equations to construct the entire distribution. This relies on the assumption of a Gaussian distribution as a first approximation. For increased resolution, discussion is given into how a path integral solution may be incorporated. Our findings highlight the important role of stochastic atomic fluctuations on the evolution of helium-vacancy cluster size distributions. The model is formulated in a general way, capable of including point defect drift due to internal temperature and/or stress gradients, which in practice arise from such issues as pulsed irradiation and both externally applied stresses or internally generated non-homogeneous stress fields, respectively. Discussion is given into how the stochastic terms may be modified to include additional physics governing the evolution of bubbles in irradiated materials and how the model can easily be extended to include full spatial resolution.

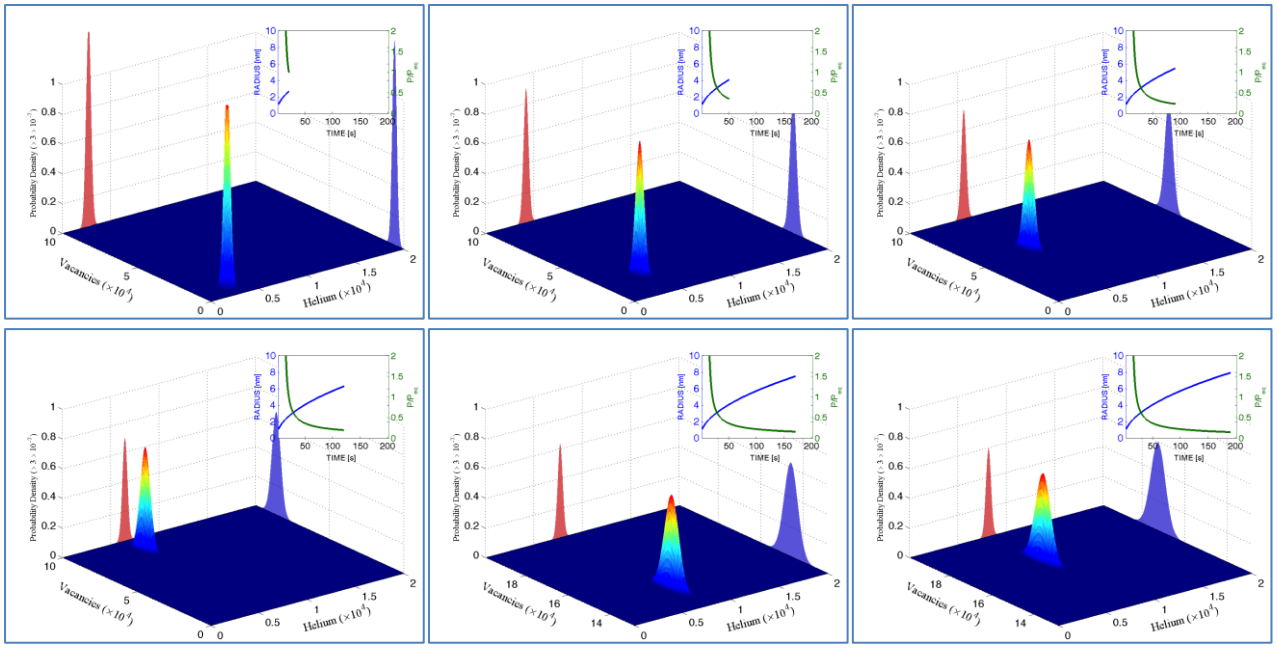

Figure 1. Evolution of the helium-vacancy size distribution spanning the first 200 seconds of irradiation time. The distribution is normalized by an arbitrary value ($3X10^{-7}$ for plotting purposes. Projections of the vacancy and helium profiles of the distribution are seen in blue and red, respectively, and the mean bubble radius and equilibrium bubble pressure ratio, are plotted in the inset plot on the left and right ordinate axes, respectively.

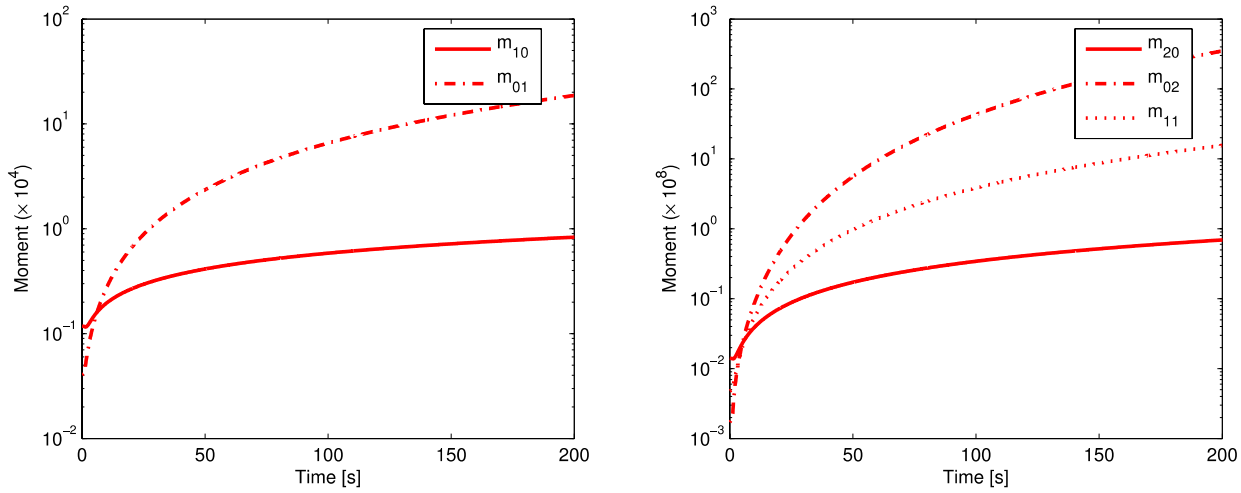

Figure 2. Log-scale plot of the moments of the size distribution versus time spanning the first 200 seconds of irradiation. The first order and second order moments are shown in the left and right plots, respectively.

REFERENCES

[1] K. Ito, Proc. Jap. Acad. Series A, 20 (1944) 519-524.
[2] N. M. Ghoniem, J. N. Alhajji and D. Kaletta, J. Nucl. Mater., 136 (1985) 192-206.