FORMATION OF SELF-ORGANIZED NANOVOIDS IN A SOLID DUE TO SURFACE STRESS AND ELASTIC INTERACTIONS

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Self-organized periodic array of nanovoids have received considerable attention in recent years for the potential in nanofabrication. The first discovery of the phenomena went back to J.H. Evans. Subjected to continual irradiation of neutrons or heavy particles at elevated temperatures, vacancies emerge in molybdenum and agglomerate into voids. These voids form a three dimensional b.c.c lattice structure, replicating the crystal lattice of the host material. The axes of the void superlattice are parallel to those of the host crystal. The ordered voids have diameters around 5~7 nm and lattice spacing around 20~30 nm. Similar phenomena have been experimentally observed in several material systems, including metals such as W, Nb, Ni, alloys such as Mo-Ti, Ni-Al, Cu-Ni and compounds such as CaF2 and NaCl. Other type of self-ordered defect clusters has also been reported. For instance, after relatively low dose of irradiation on copper and nickel, the vacancy regions form well aligned labyrinth-like defect walls. These walls are parallel to the close-packed directions of the host crystals. Despite the difference in the appearance, similar underlying mechanism may be invoked to explain the self-organization behavior.

This paper develops a model that considers both elasticity and the dynamic diffusion process [1,2]. Experiments and analytical studies highlight two observations. One is phase separation. A pure metal phase separates into two phases under irradiation: a vacancy-rich phase and a phase rich in the interstitial atom. In other words, the irradiation provides enough activation energy to induce a type of spinodal decomposition. The other one is anisotropic diffusion, which causes vacancies to accumulate at certain ordered positions. We find that it has close relation to the elastic anisotropy. We adopt a phase field approach in our model. The application of a diffuse interface allows voids to emerge or dissolve naturally, and the system can form whatever lattice it favors. Voids are treated as high vacancy concentration regions. Dynamic processes, such as void coalescence, are captured by updating the concentration profile over time. Elastic effects due to the existence of vacancies are calculated by the microelasticity theory. We incorporate the free energy of mixing, interfacial energy and elastic strain energy into the driving force for vacancy diffusion. The simulations suggest that the elastic anisotropy can induce orientational preference in vacancy diffusion, even if the diffusivity is isotropic. It is found that vacancies migrate faster along the elastic compliant directions. This causes the self-assembled voids to replicate the host crystal symmetry. Our model suggests that self-ordering may occur only when voids/bubbles are close enough to within each other's elastic influence range. Thus a certain void/bubble density is required to form superlattice. This might explain the existence of a threshold of irradiation dose for void/bubble lattice formation. External loadings are influential to the patterns of void/bubble superlattices, according to the simulations. Together with the elastic misfit, the external loadings contribute to the elastic chemical potential. This implies that the morphology and size of nanoscale voids/bubbles can be tuned by altering the loading conditions.

References

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