Interactions Between Energetic Beams and Polycrystalline Solids

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ABSTRACT

The understanding of interaction between energetic beams and materials is of great technological importance. Energetic beams could either hinder or facilitate design of engineering components. By introducing defects in the bulk of metals, radiation of particle beams could cause changes in dimension and mechanical properties of the material. During physical vapor depositions, inclusion of energetic particles – such as in ion beam assisted deposition (IBAD) – enables the design of dense films without high thermal budget. In this PhD project, we study the interaction of energetic particles with bulk polycrystalline materials (radiation damage) and surface of polycrystalline materials (thin film deposition).

First, a lattice kinetic Monte Carlo (kMC) based simulator – ADEPT – is developed for this study. The simulator is capable of representing polycrystalline face-centered cubic solids in three dimensions, and the time scale of the simulator is on the order of seconds, which are comparable to realistic laboratory time scales. In addition, the simulator is capable of treating both the radiation process and thin film depositions.

Based on kMC simulations, this thesis reports an anomaly in the dependence of radiation-induced vacancy accumulation on grain size in polycrystalline solids. Contrary to the conventional wisdom that small grains accumulate fewer defects in bulk, the vacancy concentration is higher in smaller grains during a transient state. The origin of the appearance and disappearance of this anomaly is the competition between two atomic processes: vacancy-interstitial recombination and grain boundary absorption of vacancies. Vacancy-interstitial recombination dominates during the transient sate and results in higher vacancy concentration in small grains. Grain boundary absorption of vacancies dominates at long time scale such that vacancy concentration is lower in smaller grains after the transient anomaly. Calculations based on conventional rate theory confirm the existence and the atomistic mechanism of this anomaly.

A new mechanism of stress control in polycrystalline thin film deposition is proposed and demonstrated to be feasible by our kMC simulations. Based on Cu/In/Cu

system, our work suggests that the compressive stress that develops during thin film deposition can be reduced by use of surfactant. The origin of the effect is that surfactant In atoms effectively reduce the diffusivity of Cu adatoms on the surface, such that fewer adatoms diffuse into grain boundaries. The significance of the effect of surfactant under different deposition conditions is then discussed.