Surface/interface segregation and grain boundary diffusion under stress

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Segregation plays a critical role in many aspects since the properties of functional thin films are surface-sensitive and depend on the composition of thin films, such as the conductivity and interfacial resistance, catalysis, strength and ductility. On the other hand, it had been shown that stress can affect dramatically the performance, reliability, and durability of film-fabricated devices by changing the component distribution in thin films. Upon film fabrication, large intrinsic stress could be developed due to the broken bond on surface or at interface. Upon surface and interface segregation, diffusion-induced stress could be generated due to difference in atomic size. A general model is developed for describing the kinetic/equilibrium segregation in stressed ultrathin alloy films deposited on inert substrates (see Fig. 1).

It has been well established that grain boundary (GB) diffusion plays a critical role in many cases, such as various solid-state reactions, diffusion-induced grain boundary migration and so on. Further, the fast diffusion along GBs can easily destroy the performance of electronic devices. And the diffusional flow by GB transport under stress will also leads to the creep of a polycrystalline film. The influences of the diffusion-induced stress due to the difference in the radii of elements in an alloy and the intrinsic stress originating mainly from the surface or other kind of external stress, on the grain boundary diffusion are evaluated (see Fig. 2).

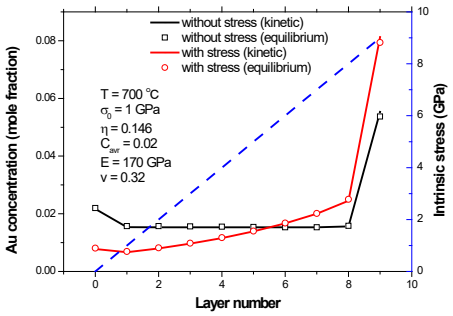

Fig. 1. Au kinetic and equilibrium concentrations for Ni(111)-2at%Au thin film with and without stress as a function of layer number.

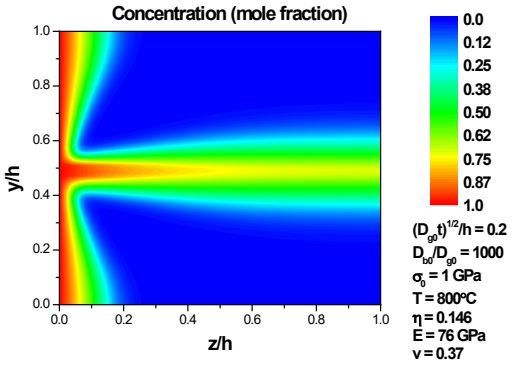

Fig. 2 The concentration profile of the Ag/Cu bilayered system under intrinsic stress and diffusion-induced stress.