Modeling of Stress Evolution during Thin Film Deposition

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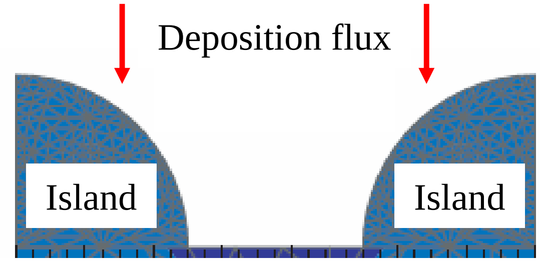
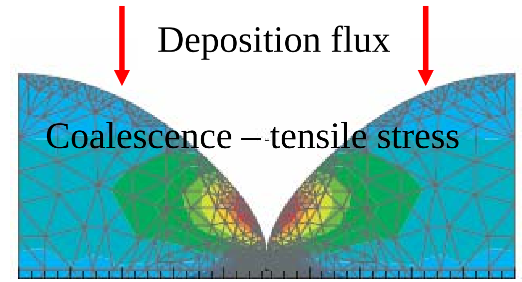
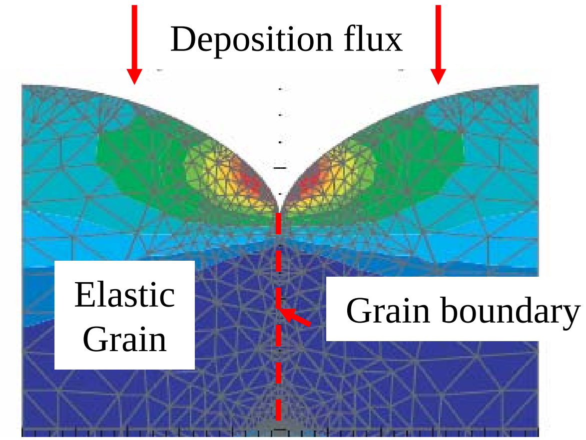
Controlling the stresses that develop in thin films during their deposition is critical to the manufacturing of reliable microelectronic circuits, as well as to coatings that are used to protect mechanical and structural components against mechanical or environmental damage.

Researchers at Brown are using computer simulations to study stress evolution during deposition of thin film materials. Previously, experiments have shown that the stress depends on the rate of growth, temperature, and thickness of the film, and can change from tensile stress to compressive stress during growth. To understand the fundamental mechanisms for generating stress, and to eventually help design deposition processes that can control stress, a new computer model has been developed to predict the evolution of stress and microstructure as a thin film is deposited on a substrate. The simulations show that there are three stages of growth. During the first stage, the film consists of isolated islands and is stress free. With further deposition, these islands coalesce to form a continuous film. At the point of coalescence, neighboring islands exert forces on each other, and develop tensile stresses in the film. As the film increases in thickness and the islands grow together, a grain boundary forms between the islands. Excess atoms from the deposited material can accumulate in this boundary, which causes a transition to compressive stress. The simulations show that the stress state is due to a kinetic balance between the mechanisms responsible for generating tensile and compressive stress. The simulations can predict the influence of growth conditions, such as the deposition rate and temperature, on the stress. Consequently, they can be used to identify growth conditions that tend to minimize stresses. This will be particularly helpful in efforts to develop ultra hard ceramic, diamond or nanocrystalline metallic coatings, which often fail as a result of the formation of severe tensile stress during growth.



Pre-coalescence – no stress





Post Coalescence – compressive stress