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Adatoms, Grain Boundaries, and Thin Film Growth Stress EDMUND WEBB III, Sandia National Laboratories, STEPHEN FOILES, CHUN-WEI PAO, DAVID SROLOVITZ, JERROLD FLORO — Atomistic simulations will be presented revealing fundamental stress generation mechanisms during later stages of thin film growth when substrate coverage is complete and the film is thickening. Typically, films exhibit texture with grain boundaries intersecting the surface. In situ growth stress experiments reveal compressive stress generation during this stage; if growth is interrupted, experiments show a relaxation in compressive stress with a characteristic rate. An existing theory proposes that, during deposition, adatoms incorporate into grain boundaries, generating compressive stress. However, debate exists regarding this mechanism and data observed in growth interrupt experiments. Simulations will demonstrate that adatoms are strongly attracted to grain boundaries and readily incorporate into them. Furthermore, adatom incorporation generates compressive stress in accord with experiments. A model is presented establishing a quantitative link between adatom incorporation into grain boundaries and the resultant stress generated.

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