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Thin film growth and mechanics: The Minimum Energy Atomic Deposition method

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Abstract

Thin-film growth is an area of research concerned with complex phenomena happening at atomic scales. Therefore, molecular simulations constitute an important tool to confront experimental results to theoretical assumptions. However, the traditional thin film growth simulation methods, i.e., Molecular Dynamics (MD) and kinetic Monte-Carlo (kMC) and combinations thereof, suffer from some intrinsic limitations, i.e. limitations in system size and simulation time for MD and predetermined reaction rates and reaction sites for kMC. Consequently, it is practically impossible to simulate the evolution of polycrystalline growth resulting in ≈100 nm thick films with realistic stress fields and defect structures, such as grain boundaries, stacking faults, etc. This contribution presents an extremely simple and computationally efficient atomistic simulation method (Minimum Energy Atomic Deposition: MEAD) to simulate thin-film deposition [1]. The method aims to overcome the limitations of existing methods to enable in-depth studies of atomic growth mechanisms, the evolution of crystal defects, and residual stress build-up during thin-film deposition—an important and active research area. The method allows depositions of tens of millions of atoms at near-equilibrium deposition rates in reasonable computational time while allowing for the growth of >100 nm-thick films with high crystallinity and low defect concentration. This has been validated on three material

systems (the deposition of Al on Si, Al on Al, and Si on Si), demonstrating that the method is much faster than MD simulations. However, the proposed method does not aim to replace the existing algorithms such as MD or kMC, but instead, improve upon the existing methods in certain aspects by integrating them into the MEAD method. One can combine the MEAD algorithm with existing techniques such as energy minimization with FIRE, thermal equilibration with tfMC, and MD equilibration, thereby also incorporating the capabilities of these techniques. Unlike on-lattice kMC, the method does not need pre-determined reaction rates and deposition sites—both of which naturally emerge from the simulation methodology. The presented results are also coherent with the experimental literature on thin film deposition. Hence, this method can be broadly used to simulate and analyze the evolution of defect structures and the build-up of residual stress during thin film growth and subsequent heat treatments. The use of in-built functions in LAMMPS makes the method easily accessible to the community.

Keywords:

Thin film mechanics Atomic deposition Residual stress

References:

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