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Stress at the initial stage of growth for Lennard–Jones films

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Keywords

film growth, stress, molecular dynamics simulation

Abstract

Molecular dynamics simulation was used to study the influence of a relative size of adsorbed and substrate atoms on the stress of growing films. Atoms in the system interact via the Lennard-Jones potential. The simulations were performed at a fixed value of systems temperature. The relative size of deposited atoms was changed in the range from 0.7 to 1.2, relatively to the size of substrate atoms. Proposed modeling allows to explain the behaviour of mean biaxial stress for systems with different sizes of adsorbed atoms and a substrate. For considered systems, significant changes in mean biaxial stress have only first three monolayers.