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Molecular dynamics simulation of temperature effects on deposition of Cu film on Si by magnetron sputtering

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Abstract The temperature effects on the growth of Cu thin film on Si (001) in the context of magnetron sputtering deposition were systematically studied using molecular dynamics (MD) method. To improve the comparability of simulation results at varying temperatures, the initial status data of incident Cu atoms used in all simulations were read from an identical file via LAMMPS-Python interface. In particular, crystalline microstructure, interface mixing and internal stress of Cu thin film deposited at different temperatures were investigated in detail. With raising the substrate temperature, the interspecies mixed volume and the proportion of face-centered cubic (fcc) structure in the deposited film both increased, while the internal compressive stress decreased. It was found that the fcc structure in the deposited Cu thin films was <111> oriented, which was reasonably explained by surface energy minimization and the selectivity of bombardment energy to the crystalline planes. The quantified analysis of interface mixing revealed that the diffusion of Cu atoms dominated the interface mixing, and the injection of incident Cu atoms resulted in the densification of phase near the film-substrate interface. More important, the distribution of atomic stress indicated that the compressive stress was mainly originated from the film-substrate interface, which might be attributed to the densification of interfacial phase at the initial stage of film deposition.

Keywords: Molecular dynamics method; Magnetron sputtering; Temperature; Crystalline structure and orientation; Atomic-level stress; Interface mixing.

Introduction:

The growth of Cu thin film on Si substrate has been intensively studied due to its potential application as interconnecting material in Si ultra-large scale integrated (Si-ULSI) devices [1], buffer layer [2], and catalyst [3]. In addition, Cu/Si interface has also received considerable attention for its application in photo detectors [4] and chemical sensors [5]. Various methods have been employed for the growth of Cu/Si thin film, such as molecular beam epitaxy [6], electron beam evaporation [7], atomic layer deposition [8] and magnetron sputtering [9]. Among these techniques, magnetron sputtering deposition has attracted great interest owing to its higher productivity and lower manufacturing cost. The performance of sputtered film is determined by various deposition conditions, among which substrate temperature is a major one that can influence the crystalline structure [10], interfacial strength [11] and internal stress [12] of deposited thin film. Synthetic investigation on these temperature effects is necessary for determining the optimal parameters to fabricate high-quality sputtered films. However, because of the limitation of experiment conditions, current experimental studies tend to focus on only one specific aspect, thus can hardly provide comprehensive understanding. Molecular dynamics (MD) method as an alternative approach is well suited to systematically characterize these temperature effects at atomic scale.

In the past few years, MD simulations have been performed to investigate the growth of Cu/Si thin films via electron beam vapor deposition [13, 14] and cluster deposition [15, 16]. However, the MD simulation of film deposition by magnetron sputtering has been rarely reported, which may be partially due to the complicated transport processes of sputtered particles. Chu and Chen [17] adopted MD method to study the growth of Cu film deposited on Cu substrate by sputtering deposition under