Deposition and growth of the AlCoCuFeNi high entropy alloy thin film: molecular dynamics simulation

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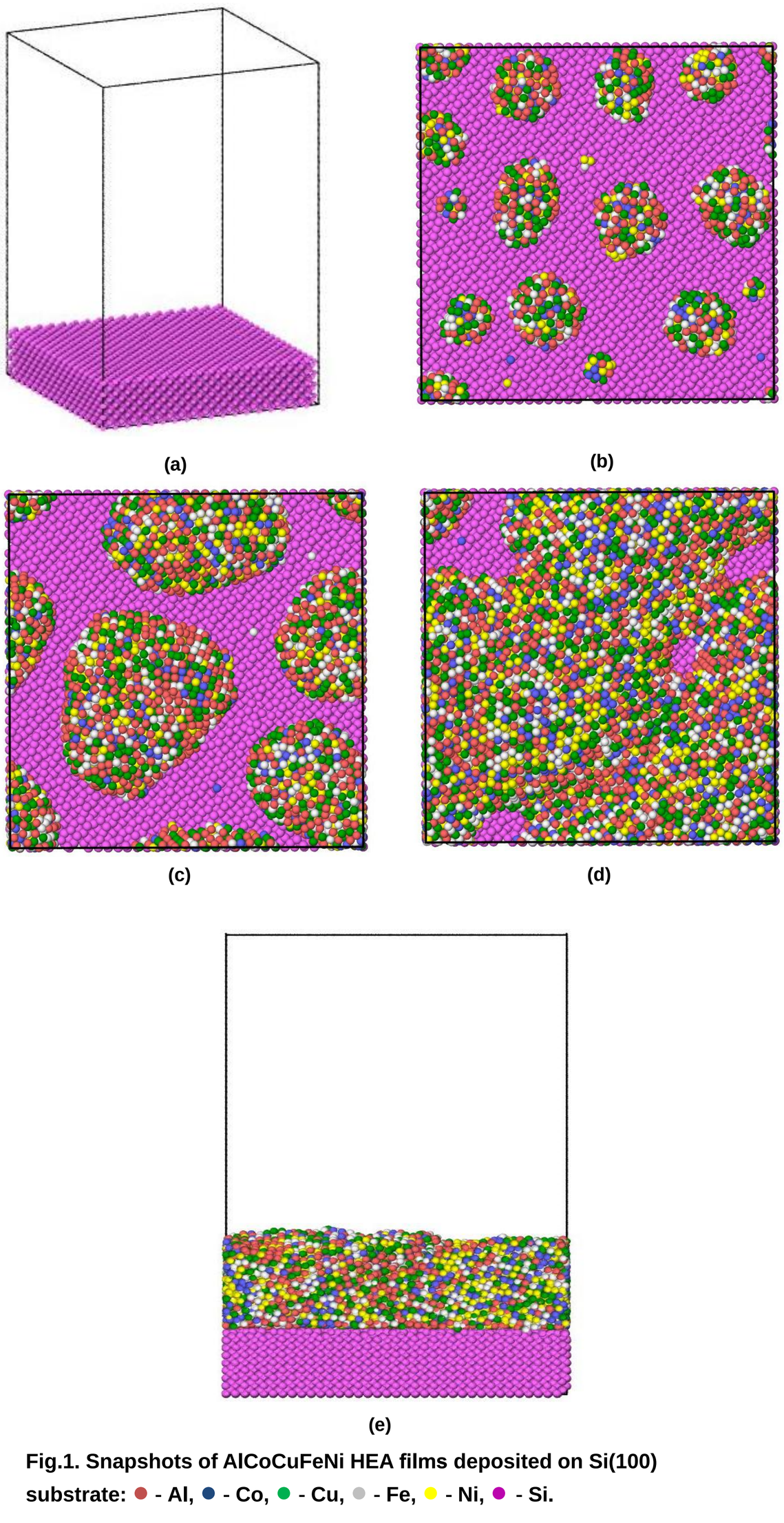
Introduction

High entropy alloys (HEAs) are relatively new class of metallic materials developed by Yeh et al. in 2004. Such alloys usually contain from 5 to 13 major elements in equiatomic or near equiatomic concentrations (5 to 35%). Due to the high mixing entropy, multicomponent high entropy alloys typically consist of simple solid solutions with a BCC or FCC lattices. The majority of HEAs were investigated in the as-quenched or homogenized state, whereas much less attention was paid to the study of thin films of high-entropy alloys. However, HEAs are sometimes difficult to synthesize as bulk materials because very fast cooling rates are required to avoid the formation of complex crystallized phases and to freeze low ordered structures. Understanding the growth mode of complex multielement HEA films is an important research topic. In this work, the processes of deposition and growth of thin films of AlCoCuFeNi HEA on the surface of monocrystalline silicon substrate were investigated by classical molecular dynamics (MD) simulation using the LAMMPS software package.

Simulation model and methods

The simulation was carried out using the embedded atom model (EAM), the interaction between the silicon atoms was described using the Stillinger-Weber potential, and the interaction between the atoms of Al, Co, Cu, Fe, Ni, and the substrate was modeled using the Lennard–Jones potential. Classical MD simulation studies of deposition and growth of thin films of AlCoCuFeNi HEA have been performed using Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS, Sandia National Laboratory, USA). Visualization of snapshots and the coordination analysis are done using open visualization tool software OVITO. A three-dimensional cell with periodic boundary conditions in two horizontal ***x*** and ***y*** directions was used for simulation. A free boundary condition was used in the vertical ***z*** direction to allow the surface growth. The monocrystalline silicon substrate was 10×10×2.2 nm (Fig.1a). To prevent the shift of the computational system due to the impact of the adatoms with the top surface of substrate, the positions of several bottom atomic planes were fixed. To ensure isothermal growth conditions, a substrate region above the fixed atomic planes was controlled by a thermostat and maintained at a temperature of 300 K. The atoms of metals Al, Co, Cu, Fe and Ni in the equimolar ratio were directed to a substrate with the atomic flux density of $5 \cdot 10^{25}$ at/m^2.The velocities of the deposited atoms corresponded to the mean kinetic energy of 10 eV, which was chosen in order to match at the best the deposition conditions in the modernized method of three-electrode ion-plasma sputtering technique.

Results



(a) **(b)** **(c)** **(d)** **(e)**

Fig.1. Snapshots of AlCoCuFeNi HEA films deposited on Si(100) substrate: ● - Al, ● - Co, ● - Cu, ● - Fe, ● - Ni, ● - Si.

In total 18825 atoms were deposited on the substrate, and the thickness of the formed film reached ~ 3 nm. According to the results of the simulation, it was found that in the initial stages of growth the film represents an islet-like structure (Fig.1b). Later, the growth of the islands and the formation of continuous coating begins (Fig.1c,d,e). Due to the limited number of impinging atoms, a fully continuous film is not reached. At the characteristic sizes of islands ~ 2 nm, the process of crystallization begins. In accordance with common neighbor analysis, after the 4,53 ns of modelling, the simulated film contains a face-centered cubic (FCC) phase (content 15,1%), a body-centered cubic (BCC) phase (content 21,2%), a hexagonal close-packed (HCP) phase (content 22,4%) (Fig.2) and an indefinite phase (content 41,3%), which, according to the analysis of the radial distribution of atoms, has an amorphous structure. The determined parameters of the lattice: FCC *a* = 0,3634 nm, BCC *a* = 0,2909 nm. The features of the distribution of the HCP phase atoms (Fig.2) allows us to conclude that this phase consists mainly of intrinsic (two adjacent HCP layers) and extrinsic (two HCP layers with an FCC layer between them) stacking faults in the lattice of the FCC phase. The twin boundaries between the FCC twins (a single layer composed of HCP atoms) are also present. As for the amorphous phase, its appearance can be explained by the high cooling rate at which some of the atoms have not enough time to rearrange and create a crystalline phase.

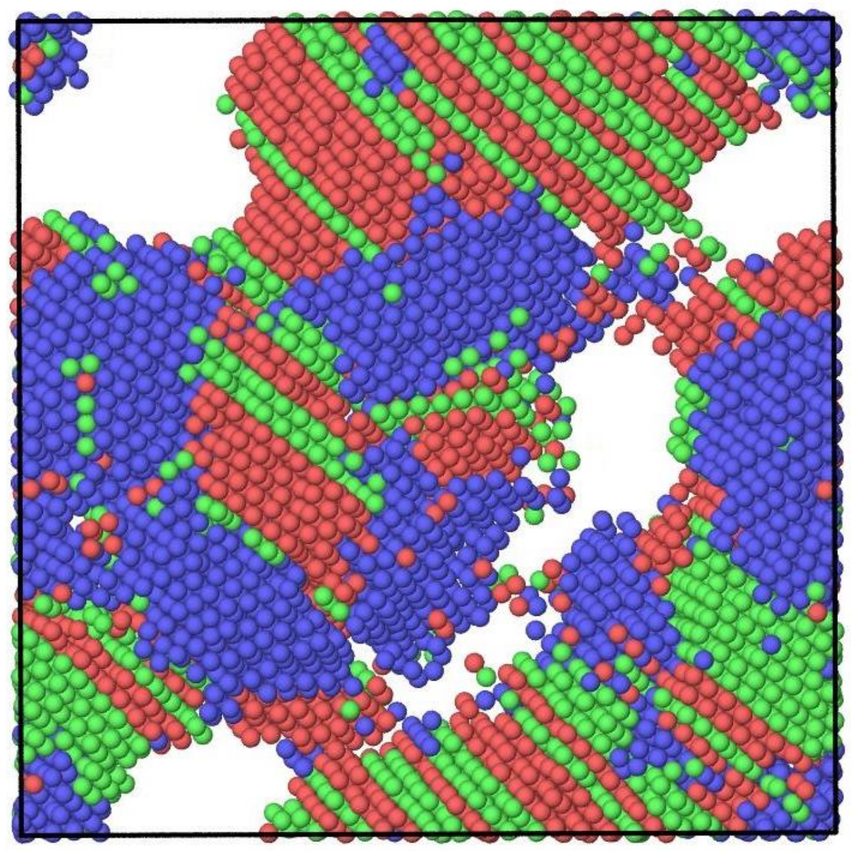


Fig.2. The common neighbor analysis (CNA) results for deposited AlCoCuFeNi HEA film (amorphous phase and substrate eliminated): ● - HCP, ● - BCC, ● - FCC.

Conclusions

MD simulations are carried out for describing initial growth of AlCoCuFeNi HEA thin films. According to simulation results, the growth of AlCoCuFeNi films occurs via a formation of three-dimensional adatom clusters or islands with subsequent coarsening and coalescence. The deduced lattice parameters of the BCC and FCC phases are in good agreement with the lattice parameters of bulk AlCoCuFeNi alloy obtained from the experiment (0.2878 and 0.3624 nm for the BCC and FCC phases respectively).