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Molecular Dynamics Simulation of Al-Co-Cr-Cu-Fe-Ni high entropy alloy thin film growth

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ABSTRACT

Molecular dynamics (MD) simulations are used to study AlCoCrCuFeNi high entropy alloy (HEA) thin film growth on a silicon (100) substrate. Effect of the atomic composition is studied on morphology and atomic scale structure. Input data are chosen to fit with experimental operating conditions of magnetron sputtering deposition process. It is observed that the different structures are determined by the chemical composition and atomic size mismatch. The simulated results are in good agreement with the solid-solution formation rules proposed by Zhang et al [1] for multi-principal component HEAs which based on the two parameters δ and Ω , respectively describing describe the comprehensive effect of the atomic-size difference in the n-element alloy and the effects of enthalpy and entropy of mixing on formation of multi-component solid-solutions. When $\Omega \geq 1.1$ and $\delta \leq 6.6\%$, the multi-component solid solution phase could form. In contrast, the multi-component alloys forming intermetallic compounds and bulk metallic glasses (BMG) have larger value of δ and smaller value of Ω . The value of Ω for BMG is smaller than that of intermetallic compounds.

Keywords: MOLECULAR DYNAMICS SIMULATION, COATINGS, HIGH-ENTROPY ALLOYS

1. Introduction:

High-entropy alloys (HEAs) have attracted increasing attentions because of their unique compositions, microstructures, and adjustable properties. Proposed by Yeh et al [2, 3], HEAs contain five or more principal elements in equal or near-equal atomic ratios, the corresponding atomic concentrations lie between 5% and 35%. Because of the high entropy of mixing, formation of brittle intermetallic phases can be avoided and simple disordered solid-solution structures like the face-centred cubic (FCC) and body-centred cubic (BCC) ones can be stabilized [1, 2]. The combination of numerous metallic elements with different sizes induces a sluggish atomic diffusion, leading to nanocrystalline or amorphous structures. Bulk HEAs demonstrate superior potential for engineering applications [4] due to their high strength [5], hardness [6], wear resistance [7], high-temperature softening resistance and oxidation resistance [8]. HEAs can be viewed as atomic-scale composites; their final properties come from: 1) the combination of properties of their constituting elements and 2) the stabilized solid solutions and structures. Thus for the design of new alloys dedicated to a given application, the prediction of structural features of the material would be of particular interest.

However, it is quite difficult to synthesize HEAs as bulk materials because very fast cooling rates are required. Compared to many thin film deposition techniques, the sputtering method is an easy way to control the chemical composition, grain size, preferred orientation and hardness by varying the deposition parameters. Few studies on HEA thin films deposited by magnetron sputtering have been published [3, 9-13]. In

addition, understanding the growth mode of such complex multi-element films remains a challenging research topic. In this view, carrying out simulation of the process at the atomic level and comparing with the published literatures is of great interest. Molecular Dynamics (MD) simulations are a powerful tool in computational materials science, which can provide a deep insight into the atomic mechanism of ordering of HEA. It can reproduce such processes and provide information not accessible experimentally. In previous works [12, 13], the growth of AlCoCrCuFeNi HEA clusters and their annealing properties have been studied. Moreover, phase transition from bcc to fcc structure was evidenced by MD simulation [14, 15], in agreement with experimental results obtained on bulk or thin film alloys. In this work, we performed a deeper and more precise work on the microstructure evolution of HEA thin films grown in operating conditions corresponding to magnetron sputter deposition. First, we studied the nucleation and growth processes occurring in HEA thin film formation; Second, the conditions of solid solution formation were explored in terms of the δ and Ω , parameters typically used for the characterization of multi-components HEA materials [1].

In those simulations, the atomic interactions for the Al-Co-Cr-Cu-Fe-Ni alloy were described by an embedded atom method many-body potential [16, 17]. Tersoff empirical potential was used for describing the substrate Si-Si interactions [18, 19]. The interactions of metal atoms with silicon were described using a Lennard-Jones potential and Lorentz-Berthelot mixing rules [14]. The local atomic structures were identified and characterized by calculating the radial distribution functions (RDF) and simulating the corresponding X-ray diffraction (XRD) patterns. The time evolution of the

crystallization process was also addressed. Comparison with available experimental data confirmed the relevance of MD simulations to predict HEA thin film features.

2. Experiments:

Thin HEA thin films have been synthesized at the GREMI laboratory (Orléans, FRANCE) using DC magnetron sputtering technique with mosaic targets (patent no.WO/2008/028981). The experimental set up is widely described in reference 12. Three targets are placed in the chamber in front of rotating Si (100) substrates in order to ensure large overlapping of the sputtered atom fluxes of pure elements (99.99%). The six chemical elements are arranged on the targets (Fig. 1) [20]: Fe, Co and Ni are on target 1, Cu and Cr on target 2 and Al on target 3.

The relative surface fraction of each element on the target was calculated, taking into account the difference in sputtering yields estimated with TRIM software in order to reach the equimolar composition. However it is possible to adjust the stoichiometry of AlCoCrCuFeNi alloy in a narrow range, by varying the electrical powers applied to the magnetron cathodes independently. Note that in the present target configuration, the concentrations of elements present on the same target are linked.

Thin films of more than 1 μm thickness were synthesized on Si (100) substrates. X-ray diffraction (XRD) analysis (Cu $K\alpha$ radiation, $\lambda = 0.154$ nm, Bragg–Brentano geometry) was performed to determine the crystalline phases and the stoichiometry of the thin films was determined by Energy Dispersive Spectroscopy (EDS). In this paper three samples will be under investigation: $\text{Al}_2\text{Co}_9\text{Cr}_{32}\text{Cu}_{39}\text{Fe}_{12}\text{Ni}_6$, sample 1, $\text{Al}_3\text{Co}_{26}\text{Cr}_{15}\text{Cu}_{18}\text{Fe}_{20}\text{Ni}_{18}$ sample 2 and $\text{Al}_{39}\text{Co}_{10}\text{Cr}_{14}\text{Cu}_{18}\text{Fe}_{13}\text{Ni}_6$ sample 3.

3. Simulation details:

MD simulations for the present HEA system were carried out in a three dimensional cell. Periodic boundary conditions were used in two horizontal x and y directions so that the simulated systems could be viewed as large planes in the x-y dimension. A free boundary condition was used in the vertical z direction to allow for surface growth.

The substrate is Silicon (100) with dimensions of $10a \times 10a \times 5a$. a is the Si lattice parameter, i.e. 5.4308 Å. The velocities of the deposited atoms are sampled from a Maxwell-Gaussian distribution with a most probable energy of 1 eV, and with randomly selected incident angles. The mean kinetic energy of 1 eV was chosen in order to match at the best the deposition conditions in magnetron sputter technique at low argon pressure., it simulates sputtering experiments at low argon pressure where a small amount of buffered gas only randomizes sputtered atom velocities without not too much energy loss The deposition model of the six atoms is shown in Fig. 2. To prevent the shift of the computational system due to the impact of the adatoms with the top surface, the positions of four bottom atomic plane of atoms (depth a) were fixed during simulations. Besides, the system temperature will rise due to kinetic energy released by impinging atoms. To mimic isothermal growth conditions, an intermediate region above the fix region (depth $2a$) is controlled by a Berendsen thermostat and maintained at a desired substrate temperature (here 300K). Atoms located in the surface region (thickness $2a$) are left free to move and thus are able to respond to incoming atom impacts.

During MD simulation, 15000 atoms are released to the Si surface for realizing the three

deposition sets. Table 1 gives the number of atoms really living in the simulated film and the corresponding composition. The sticking coefficient is found close to 0.9 and the compositions of the simulated samples are closed to the targeted ones.

After simulation, radial distribution functions (RDF) were used to employ the correlation between the atoms and the simulated powder X-ray diffraction patterns (XRDs) to analyze the phase of HEA thin film. The simulated XRD patterns were determined by using Debye functional analysis as described in detail by Kazakov and co-workers [21]. I is the intensity of the diffracted coherent radiation and is determined by the Debye formula.

$$I_k(b) = \sum_n \sum_{n \neq m} f_n(b) f_m(b) \frac{\sin(2\pi b r_{nm})}{2\pi b r_{nm}}$$

where $b=2\sin(\theta)/\lambda$ and λ is the wavelength of the incident radiation, 2θ is the scattering angle, and r_{nm} is the distance between atoms n and m . The functions $f_n(b)$ and $f_m(b)$ are the scattering factors for atoms n and m , respectively.

4. Results and discussions:

Simulation snapshots for sample1-3 thin films are displayed in Fig. 3. It is clear that the atoms, in sample 1 and sample 2, are arranged in a crystalline structure. For sample 3, however, an amorphous structure is formed on the overall thickness.

For analyzing deposit properties, first simulated and experimental XRD patterns are compared (figure 4); second, we discuss the process of HEA thin film growth (Fig. 5-7); and third, we use solid-solution formation rules to characterize the collective behavior of these three samples (Fig. 8, 9).

4.1 Determination of Simulated Powder X-ray Diffraction Patterns.

The experimental XRD θ - 2θ peaks are shown in figure 4(a). The following peak positions are observed: $2\theta = 43.81$ for sample 1 attributed to the fcc (111) β structure, $2\theta = 44.41$ for sample 2 attributed to the bcc (110) α structure and $2\theta = 43.77$ for sample 3. However, the broad and low intensity peak in sample 2 could indicate a mixture of both solid solutions and a less ordered phase.

The calculated X-ray intensities vs. 2θ of simulated HEA thin films are shown in figure 4(b). By comparing both XRD plot sets, it can be observed that the peak positions in the simulated XRD are close to that detected in the experimental XRD patterns (see table 2). The simulated peaks at positions $2\theta = 43.97^\circ$, 44.57° and 42.50° correspond to samples 1~3 respectively, sample 2 being close to the bcc(1 1 0) α structure while sample 3 peak is fairly consistent with fcc (1 1 1) β [22]. In this latter case, because the peak is broader than for Sample 1 and 2, the structure has a much shorter range order, in agreement with the amorphous-like snapshot of this sample. While, the peak intensities are very different between simulations and experiments.

It is important to note that it is not possible to directly compare intensity and width of experimental XRD peaks to that of simulated ones. The FWHM of XRD peaks depends on the size of crystalline domains, which of course are larger on 300 nm thick HEA films than on simulated films composed of a limited number of atoms (1500 in our case). Thus the total number of atoms participating to the diffraction pattern is completely different. The relative intensities of the peaks are also related to the crystalline quality. It appears from Fig. 4 that experimental S2 and simulated S3 samples exhibit a worth crystallinity than the others. This difference between experiment and simulation

remains unexplained but may be attributed to the experimental conditions (energy flux transferred to the surface during the growth for example) that were not exactly during the synthesis of S1, S2 and S3 samples.

4.2 The growth process of the HEA thin film

Examination of the snapshots, as displayed in Fig. 5a-① to 5a-⑥, at different times, shows the growth of $\text{Al}_2\text{Co}_9\text{Cr}_{32}\text{Cu}_{39}\text{Fe}_{12}\text{Ni}_6$ thin film deposited on Si (100) substrate. At first step ($t = 0.5$ ns), it is found that small clusters are formed, which leave the substrate partly uncovered. As the number of deposited atoms increases, a continuous film is formed (from 2.5 ns). It can be clearly seen that the structure is amorphous on the first two snapshots of Fig. 5a, which is also evidenced on the RDF plotted in Fig. 5b. The RDF curve is relatively smooth and does not exhibit any defined peaks at expected bulk crystal neighboring positions shown in table 3. Those positions have been calculated from element crystal values found in reference 14 and are given here for equimolar composition. The RDF shape lies between a crystal and liquid indicating an amorphous structure. Going on with the deposition process, when more atoms are released onto the substrate, the RDF patterns change a little bit: the first peak (at 2.52 Å) becomes narrower, the second peak (above 4 Å) splits and a new peak at $r \approx 2.84$ Å gradually arises. This indicates that the thin film changes from amorphous to crystalline structure. This phenomenon can also be observed in Fig. 5a. At ≈ 3.5 ns to 6.0 ns. First, grains with crystallized structure are formed on the top of the film (see Fig. 5a-③). Then, new grains nucleate at locations close to the existing ones. Finally, this process propagates across the thin film leading to a single-crystalline structure (see Fig. 5a-④).

It is found that the emergence and growth of a critical nucleus plays a key role in the crystallization of the HEA film alloy. The critical nucleus triggers a strong spatial correlation with other crystal nuclei in its surroundings just before the onset of crystallization, which may provide a subsequent rapid crystallization.

The snapshots of sample 2 deposited on Si(100) substrate at different stages are shown in Fig. 6a. It is obvious that sample 1 and sample 2 exhibit the similar final product of magnetron sputter deposition, i.e. a crystallized film (shown in Fig. 5a-⑥ and Fig. 6a-⑥). However, the drastic difference can be observed in the growth process of both alloys. For sample 2, at 2.5 ns, various crystalline clusters with same lattice orientation are formed on the Si(100) substrate (shown in Fig. 6a-②), while for sample 1 a continuous amorphous film is observed (shown in Fig. 5a-②). These results are consistent with the RDF analysis. It is seen that at 2.5 ns RDF patterns features of sample 2 are typical of a crystallized film: narrower first peak, appearance of a peak at 2.84 Å and splitting of the second peak. This implies that the film in sample 2 has the strongest ability of crystallization, which could only be correlated to the chemical composition. It seems thus, that the atomic size difference has significant effect on the film structure. After several crystalline clusters have been formed, they grow in size along the direction perpendicular and parallel to the Si(100) substrate. Interfaces between adjoining clusters of various orientations are formed. Finally, the different crystalline cluster join together. In order to reduce the energy of the system, the structure of the sample rearranged and the direction of the lattice rotated. This is depicted in the Fig. 6-③ - Fig. 6-⑥. In this simulation the energy of depositing atoms seems to be

high enough to overcome the diffusion activation energy and lead to reconstruction the film as a whole with a new lattice orientation.

Fig. 7 shows the snapshots and RDF of sample 3 at different times. Comparing with sample 1 and 2, the RDF at all times exhibits the typical features of an amorphous structure, where the first and second peak are broad and higher-order peaks fade away quickly. This is also clear on the corresponding snapshots given in Fig. 7(a). All these points indicate that sample 3 grows as an amorphous film.

RDF features can be explained by the close-packed hard ball model. The structure stabilized in multi-element alloys can be attributed to the effect of mixing numerous elements with different atomic sizes as depicted in Fig. 8. The circles represent the first, second, third, fourth and fifth shells, respectively. It is seen that a crystal structure will have many sharp RDF peaks corresponding to the first, second, third, fourth, fifth shells and so on (Fig. 8(a)).

In an amorphous structure, because of the most compact system rules, the first shell will be stable (only a change due to the presence of neighbor atoms with different atom radius could be detected). While, the second and third shells, and also the fourth and fifth shells, being quite close in space, it is expected that a certain degree of shell diffusion renders them indistinguishable from each other (Fig. 8(b)) [23]., Thus an amorphous structure exhibits a split second peak reflecting the partial merging of the second and third shells, and the third broad peak reflecting the merging of the third and fourth shells.

Following the hard ball model, atomic radii and deviation from the mean radius for

each element in the system are shown in table 4. The deviation of the mean distance of Al is much higher than other element. Considering sample 3 has the largest ratio of Al (39%), it is more easily for the second and third shells to be distinguishable and behaved as a liquid-like structure or amorphous structure (Fig. 8(b)).

4.2 Solid-solution formation rules for HEA

Currently, the phase stability of high entropy alloys has been widely investigated [1, 24-26] Among them Zhang et al [1] proposed that two parameters can be used to characterize the collective behavior of the constituent elements in multi-component (more than 4 elements) alloys: δ ($\delta = \sqrt{\sum_{i=1}^n c_i (1 - r_i/\bar{r})^2}$ where c_i is the atomic percentage of the i^{th} component, and \bar{r} is the average atomic radius and r_i is the atomic radius), describing the comprehensive effect of the atomic-size difference in the n-element alloy and Ω ($\Omega = T_m \Delta S_{mix} / |\Delta H_{mix}|$, where ΔH_{mix} is enthalpy of mixing, ΔS_{mix} is entropy of mixing and T_m is the average melting temperature for n-elements alloy), describing the effect of ΔH_{mix} and ΔS_{mix} on the formation of multi-component solid-solutions. From the values of parameters δ and Ω for multi-component alloys, a solid-solution formation rule has been proposed by Zhang et al. When $\Omega \geq 1.1$ and $\delta \leq 6.6\%$, the multi-component solid solution phase could form. In contrast, for larger value of δ and smaller value of Ω , intermetallic compounds and bulk metallic glass(BMG) are formed. The value of Ω for BMG is smaller than that predicted for intermetallic compounds.

The parameters of the three samples grown by MD simulations are calculated, listed in table 5 and mapped in Fig. 9. The values of δ (2.28 %, 2.89 %) and Ω (2.794, 38.986)

of sample 1 and 2 lies in the area where the formation of solid solutions is predicted. Sample 3 with $\delta = 5.94\%$ and $\Omega = 2.595$, stays in the overlap area of “Solid Solutions” and “Intermetallics”, which indicates both solid solutions and intermetallics are likely to be formed. Thus, solid solution could be predicted to form in all samples, and ordered intermetallics could also appear in sample 3, for which parameters tend to enter the metallic glass zone. However, the simulation results shown in Fig. 3 evidence that, crystalline structures are just observed in sample 1 and 2, and do not appear in sample 3. The sole amorphous structure formed in sample 3 could be ascribed to a kinetic factor. It is well known that deposition by magnetron sputter technique could lead to the formation of metastable phases. With no external heating of the substrate, low ordered phases are usually obtained. The solid solution formation rules as defined from δ , Ω graph, is based on thermodynamics consideration, the kinetic effect is not emphasized, and non-equilibrium phase formation cannot be predicted.

Thus, the rules proposed by ZHANG apply well for conventional bulk alloy equilibrium synthesis techniques.. In the case of thin film growth, especially when deposition conditions deviate from thermodynamic equilibrium, they could only give some expected trends. For a more precise prediction of the expected phases, simulations of the deposition process, taking into account kinetic effects, as those highlighted by MD simulations, have to be implemented

5. Conclusions:

MD simulations were carried out for describing the initial growth of AlCoCrCuFeNi

HEA thin films. From the simulation results, it has been shown that the number of elements, atomic size difference have significant effects on the atomic configuration. Crystalline layer grows for low Al content (2 % and 3 %), while, pure amorphous thin film is observed for the highest proportion (39 %) of the atom which radius deviates the most from the mean one calculated for the equimolarity. By calculating the parameters δ and Ω for the reported HEAs, a tendency to evolve from solid solution to bulk metallic glasses was expected, in good agreement with the present MD simulation results.

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