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Synthesis of Shape Memory Composites by Laser Powder Bed Fusion

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This study investigates the influence of atmosphere conditions and laser processing parameters on the microstructure and phase evolution of Cu-Al-Ni shape memory alloys synthesized via laser powder bed fusion (LPBF). The experimental results demonstrated that applying a vacuum of 10^{-2} Pa significantly improved consolidation, avoiding oxide formation compared to atmospheric synthesis. Through a multi-stage thermal strategy, including pre-heating and remelting, we achieved a refined microstructure characterized by austenitic phase with embedded martensitic lamellae. XRD and SEM analyses revealed a heterogeneous microstructure, confirming effective in-situ alloying. Mechanical characterization via local microhardness testing highlighted significant variance in hardness, attributed to the interaction between the ductile copper matrix and harder intermetallic phases. Furthermore, molecular dynamics modelling was employed to correlate the observed structural features with the mechanical response of the material. These findings provide critical insights into optimizing LPBF parameters for producing high-performance Cu-Al-Ni components with tuneable functional properties.

Keywords: Cu-Al-Ni alloy, shape memory alloy, additive manufacturing, selective laser melting, laser powder bed fusion, microstructure, microhardness, functional gradient structure.

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Introduction

Materials with tunable properties cover a significant area of research, particularly in the development of composites obtained from components with different physico-chemical characteristics. By tuning the volume fraction of each component, specific functional requirements can be achieved. Nowadays, various composite materials are successfully employed in a wide range of technological applications. Another promising class of materials is functionally graded materials (FGMs), which exhibit a controlled spatial variation in composition, and has been extensively studied over the past decade. The development of these materials was initially inspired by biological systems found in nature [1,2,3]. The term "gradient materials" describes a gradual change in structural or chemical characteristics that gives materials new properties and functionalities. One of the first works that considered the creation of gradient metallic materials concerned the study of the change in the

grain size of copper from the central region of the ingot to its periphery. Importantly, such a gradient structure can provide high strength without reducing ductility [4,5,6]. The combination of strength and ductility exhibited by gradient-structured metals and alloys has stimulated efforts to improve other key properties, namely crack resistance [7], fatigue resistance [8], wear resistance [9] and corrosion resistance [10].

Materials with a gradient structure are classified according to two characteristics. The first concerns the structural gradient (grain size, thickness of lamellar phases, volumetric distribution of defects, cavities, etc.) and the second one the chemical gradient (phase distribution gradient, chemical composition gradient, distribution gradient of decomposition products of solid solutions). These materials were usually obtained by classical methods, namely thermal and mechanical treatments, as well as various surface treatments of metals and alloys. The development of additive technologies has created the opportunity to create (design) gradient

materials with both structural and chemical gradients. In particular, by varying the composition of the powder mixture and the laser processing modes, it is possible to form such materials using selective laser sintering or powder bed fusion. Therefore, the modern approach to designing elements and mechanisms is based on a departure from the concept of homogeneous materials in favour of systems with a programmable spatial distribution of properties. In this context, functional gradient materials (FGM), whose architecture allows for minimising interfacial stresses and optimising the specific strength of structures, occupy a special place. However, if traditional research in the field of FGM primarily focuses on regulating mechanical properties (hardness, wear resistance, or fracture toughness) by varying structural parameters, then a promising avenue for development is the creation of gradient functional composites (GFC). The integration of shape memory phases (SMFs) into gradient structures opens up fundamentally new possibilities for engineering. Creating a gradient in chemical or phase composition within a single product enables local control of martensitic transformation temperatures. This provides multi-stage activation or differential damping, which is critical for robotics, medicine, and aerospace applications.

The use of powder bed fusion (PBF) with mixtures of pure-element powders (in-situ alloying) instead of pre-alloyed powders enables direct control of the local chemical composition at each construction point [11]. At the same time, the complexity of the physicochemical processes during laser exposure of a mixture of Cu-Al-Ni powders, due to the high thermal conductivity of the copper matrix and the tendency of aluminium to selective evaporation, requires a detailed study of the regularities of phase composition formation and microstructural integrity. In addition, various post-processing methods demonstrate a significant impact on the functionality of the Cu-Al-Ni shape memory alloy (SMA) [12,13]. To improve surface quality and reduce micro-porosity, a laser remelting treatment has been combined with conventional selective laser melting [14,15]. Different scanning strategies were developed to modify and optimise microstructures [16,17,18].

This work aims to establish the regularities of the synthesis of shape memory phases in the Cu-Al-Ni system by the method of selective laser melting of a mixture of Cu, Al, Ni powders and to study the influence of laser

equipment parameters on the consolidation of particles and the formation of the microstructure and phase composition of the GFC.

I. Materials and Methods

The powder mixture was prepared by thoroughly mixing pure Cu, Al, and Ni powders, which were previously sifted through a 100 μm sieve. The mixture was blended in the proportions 81.6 Copper, 14.4 Aluminium, and 4 Nickel (Cu81.6Al14.4Ni4, wt%). The pure powders were mixed together in an automatic mixer for 60 min to obtain a uniform powder mixture. The resulting mixture was used for layer-by-layer selective laser melting (SLM) and sintering on a PBF substrate. A laser scanning system equipped with the nanopulsed fiber laser wavelength of 1065 nm, with Gaussian laser beam, operated at different power (P) and scanning speeds, was used for sintering the powder mix.

Figure 1 shows the scheme of the powder laser processing, where a focused laser beam scans the surface with a scanning step (Sc). A laser track width corresponds to the diameter of the beam in a focal plane. The material processing was carried out both in an air atmosphere and in vacuum 10^{-2} Pa. The scanning strategy is bidirectional scanning (back-and-forth motion), rotating the beam's motion vector by 90 degrees at each iteration. Each processing stage (pre-heating, fusion, and remelting) consisted of five iterations. Operating parameters and processing stages are displayed in Table 1.

The X-ray diffraction method (Cu-K α radiation, wavelength of 0.15418 nm) and Field Emission Scanning Electron Microscope (FE SEM) Hitachi S-4100 with a secondary electron detector was used to study the composite structure after laser powder bed fusion. The microhardness was measured using a NOVOTEST equipment. The study of the sintering process of nanoparticles was carried out by the method of Molecular dynamics using the free open package for classical molecular dynamics LAMMPS. OVITO tools were used to visualize the obtained results, which allow not only visualization of the modeling process, but also some calculations [19].

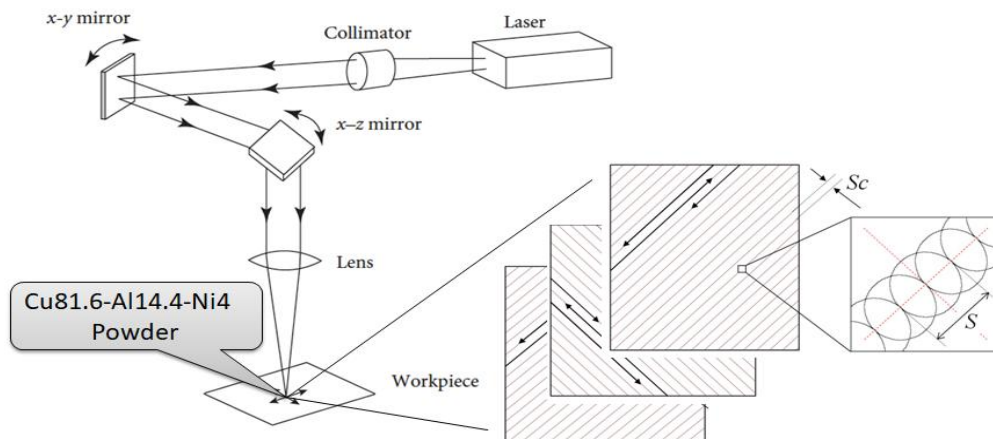


Fig. 1. Scheme of the equipment for SLM/PBF and scanning strategy.

Table 1.

Operating parameters of LPBF			
Mode	Pre-heating	Fusion	After-treatment / remelting
N	Laser power, W (Fluence, J/mm ²)	Laser power, W (Fluence, J/mm ²)	Laser power, W (Fluence, J/mm ²)
1	-	37.5	-
2	-	40.0	-
3	-	42.5	-
4	20	42.5	42.5
5	20	45.0	45.0
6	20	47.5	47.5
7	20	42.5	-
8	20	45.0	-

II. Results and Discussions

As a result of layer-by-layer sintering on a substrate by selective laser melting of the powder mixture, we obtained samples of a continuous composite material with different strengths and porosity. The X-ray diffraction (XRD) curves, shown in Fig. 2a, indicate the formation of a multiphase structure. Reflexes corresponding to copper, martensite, and high-temperature austenite ($\beta 1$) were detected. In the samples obtained at lower energy modes, CuO and Cu₂O were detected, indicating the influence of the air atmosphere on the material's structure. X-ray curves 4 and 5 show clear peaks of austenite and weak, but noticeable, peaks of martensite. The ratio of the intensity of the main peaks indicates the dominance of the austenite component in these samples (Fig 2b). The appearance of martensite reflexes in the diffraction pattern indicates a phase transformation during rapid cooling after laser heating.

Scanning electron microscopy (FESEM) of the obtained samples allowed to reveal a specific structure characteristic of the samples at the initial stages of consolidation after laser-heating. The microstructure can be characterised as a heterogeneous structure with developed surface, consisting of partially melted particles (Fig. 3). The process can be described as liquid capillary-bridge formation between solid particles occurred under laser melting [20]. Micro-bonding have formed between individual elements of the mixture (necking zones or micro-bridges) during sintering, as shown in the figures. This indicates the active occurrence of surface diffusion and local melting in the laser's thermal influence zone. The presence of micro-bridges confirms the successful initiation of monolithic alloy formation. Due to the active formation of necking zones, the structure is characterized by irregular, deep and open pores with complex, non-spherical shapes that resemble the contours of interparticle voids (Fig. 3a). This morphology is typical for synthesis with dominating of capillary forces and high surface tension of the melt [21,22]. The absence of spherical gas pores may indicate the structure formed by mechanisms of both liquid-phase and solid-phase sintering.

The described surface shows a complex balance between the laser energy and the thermophysical properties of the Cu-Al-Ni system. The high reflection coefficient and high thermal conductivity contribute to

rapid heat removal, leading to the “freezing” of the melt into discrete structure elements [23]. The resulting texture may indicate the uncompleted coalescence and significant influence of surface tension, forming a developed “coral-like” relief with a large surface area (Fig. 3). This structure is in good agreement with the results of X-ray phase analysis (Fig. 2). The presence of areas of uncompleted fusion of elements causes the presence of strong reflexes of the pure elements, while the bonding zones can be foci of the formation of an alloy with shape memory (austenite and martensite).

With increasing laser power, a more consolidated microstructure is observed (Fig. 3b and 3c), indicating a more optimal balance between the laser energy and the thermophysical characteristics of the powder. This structural state is characterized by cellular morphology with a typical cell size of about 1 μm (Fig. 4 and 5). Such a structure can be the result of the ultra-high cooling rates (10^5 – 10^7 K/s) inherent in the SLM process. In the modes 4 and 5, an increase in the material's relative density is observed due to particle consolidation, while the bridges expand and the pores acquire a more spherical shape and smaller geometric dimensions. This may indicate the formation of a stable melt pool that fills the free spaces between the powder particles. The absence of large fragments of copper powder (which correlates with a decrease in the intensity of the corresponding XRD peaks) may indicate more efficient diffusion within the melt. The dominance of the austenite peak (220) over the copper peak (111) indicates that austenite $\beta 1$ has become the main phase in the sample (Fig. 2b). Since the peak intensity in the XRD curves is directly proportional to the volume fraction of the phase, it can be considered that most of the powder mixture (Cu, Al, Ni) successfully reacted with each other, forming a phase with shape memory. So, the laser mode was sufficient to melt most of the copper particles and diffuse aluminium and nickel into them. The “residual” peak of copper (111) is probably due to the presence of the largest powder particles that did not have time to dissolve completely. The presence of pure copper allows us to consider the material as a composite with a gradient structure.

Analysis of samples obtained in the air atmosphere showed also a significant effect of oxygen on the phase composition of the Cu-Al-Ni system and on the microstructure formation. In particular, the X-ray diffraction detected the copper oxides (CuO, Cu₂O). The presence of oxide in the melt zone is considered as

destabilizing factor for the SLM process. Oxide films, and especially refractory Al_2O_3 , have a much higher melting point than the metal matrix, impairing the wetting and fusion of powder particles (which largely causes the "balling" phenomenon). We see only copper oxides on XRD, but aluminum oxide (Al_2O_3) often does not give

clear peaks (it can be amorphous or very thin). Oxidation can lead to a change in the stoichiometry of the alloy and prevents the formation of the functional austenitic phase β_1 , responsible for the shape memory effect.

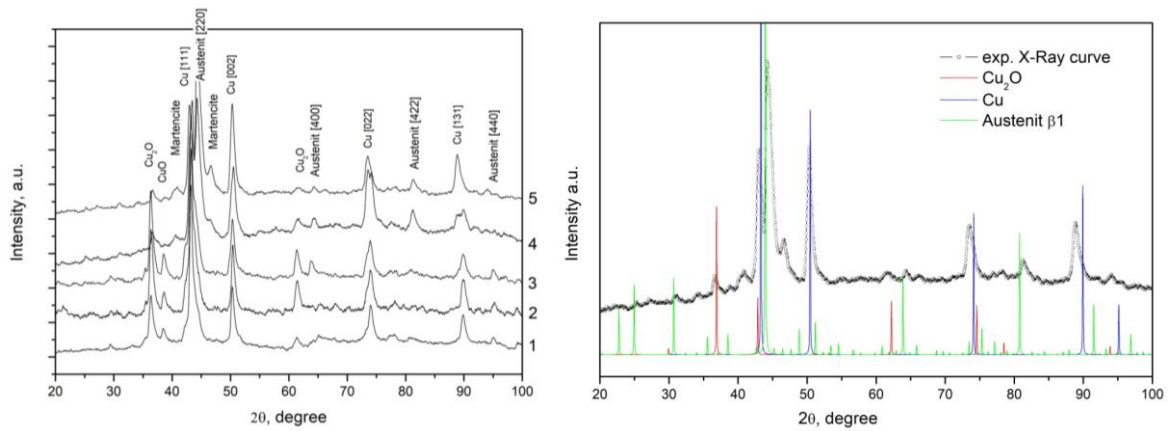


Fig. 2. X-Ray diffraction curves of samples of Cu-Al-Ni fused in an air atmosphere (a), detail analysis of curve 5 (b).

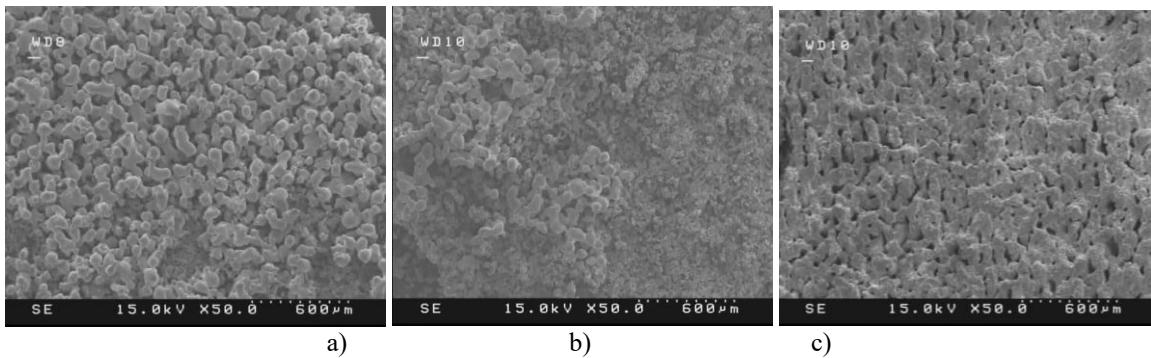


Fig. 3. FESEM images of microstructure of Cu-Al-Ni after LPBF process: a) – mode 3, b) – mode 4, c) – mode 5.

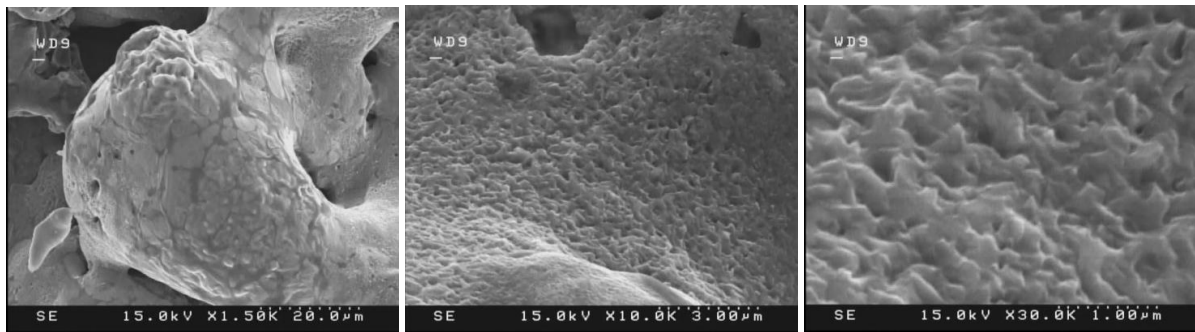


Fig. 4. FESEM images of the bridges surface (mode 2).

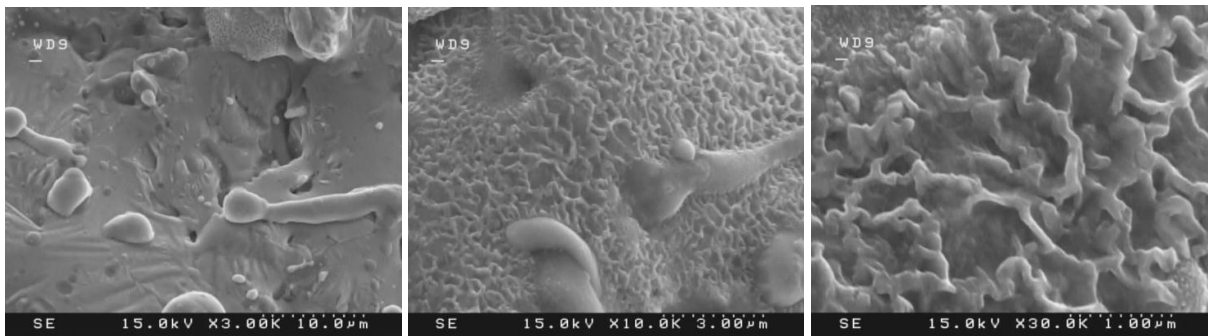


Fig. 5. FESEM images of cellular microstructure (mode 5).

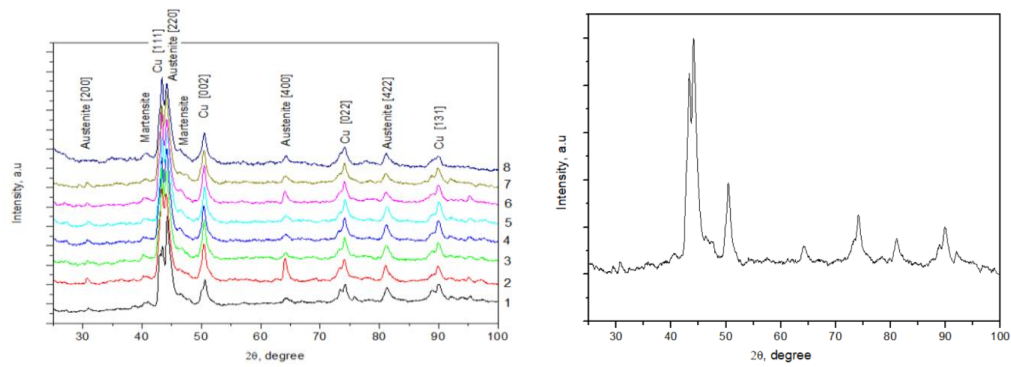


Fig. 6. X-Ray diffraction curves of samples of Cu-Al-Ni SLM fused in vacuum (a), detail analysis of curve 7 (b).

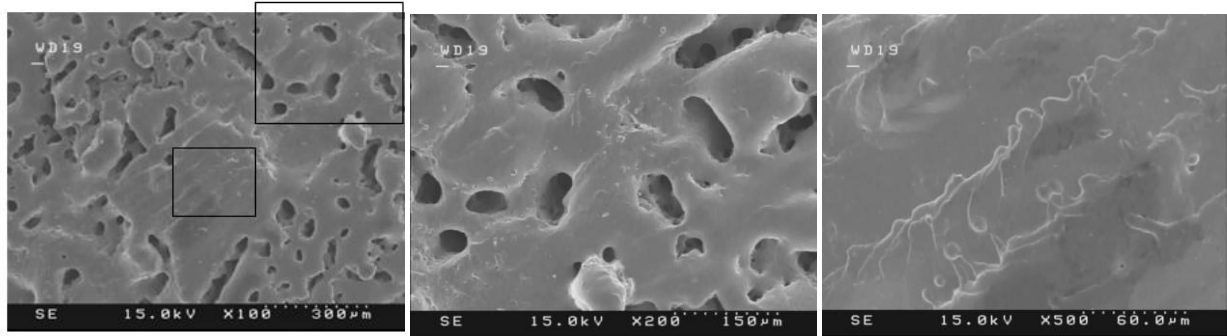


Fig. 7. FESEM images of porous microstructure of Cu-Al-Ni after SLM process in vacuum (mode 3).

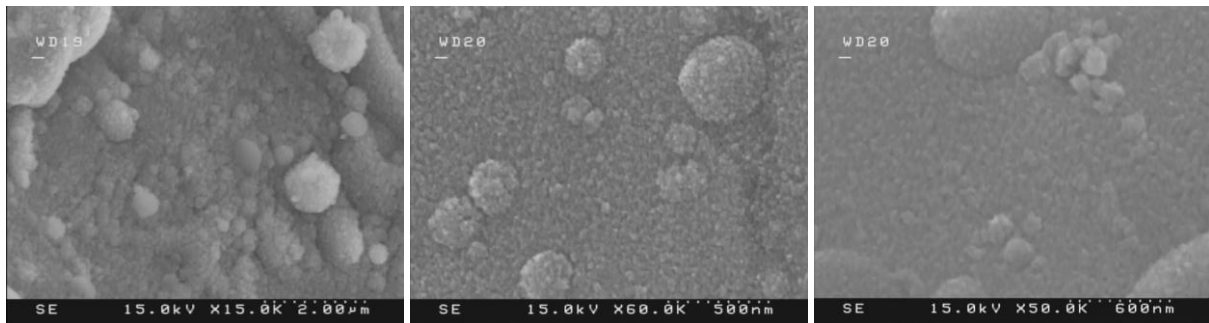


Fig. 8. FESEM images of nanostructured surface of a sample.

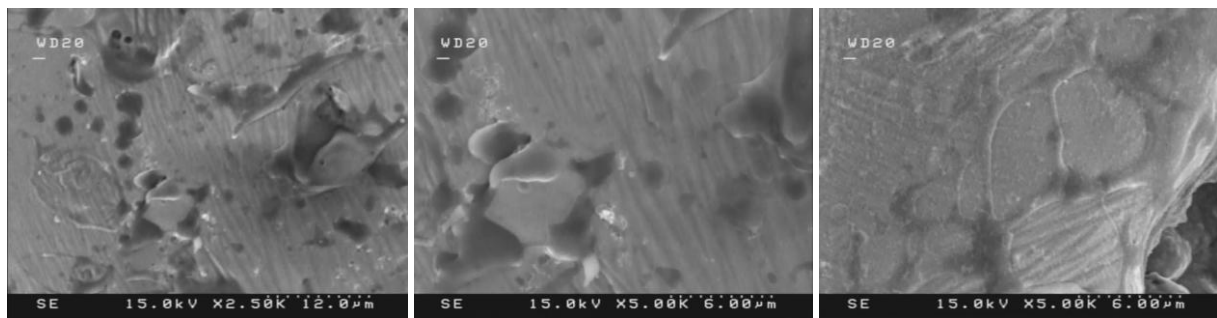


Fig. 9. FESEM images of lamellar structure.

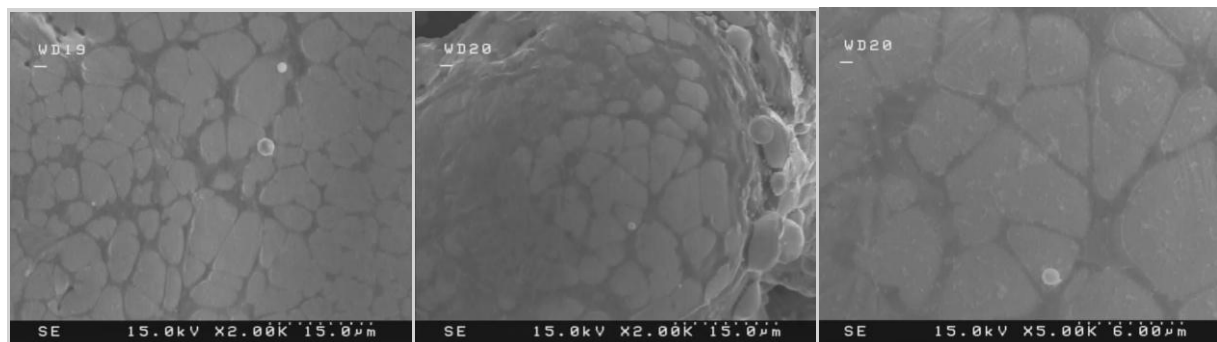


Fig. 10. FESEM images of surface microstructure.

The next stage of the study was to carry out the synthesis in an oxygen-free environment (vacuum chamber with a pressure of 10^{-2} Pa) to avoid the influence of atmospheric gases on the dynamics of the melt. FESEM analysis of the microstructure of samples synthesized in vacuum revealed a slight increase in material consolidation compared to synthesis in air. The balling effect is still observed; however, fusion zones with pronounced laser tracks are clearly visible on the sample surfaces. The use of an additional remelting stage contributes to reducing porosity. In particular, on the surface of the sample (Fig 7) a decrease in the size of the pores to 5 - 10 μm and their acquisition of a more spherical shape is observed. At the same time, the microstructure is heterogeneous, which is represented by both zones with a nanograin structure with an average grain size of less than 50 nm (Fig. 8) and areas with a characteristic martensitic structure [23,24,25], which is found mainly on the bridges (Fig. 9), and granular structure (Fig. 10). X-ray diffraction analysis revealed intense reflections from the austenite phase and pure copper, and in some samples, the intensity of the austenite peaks exceeded that of the copper matrix (Fig 6a), indicating the effectiveness of in-situ alloying. Weak but clear peaks of the martensite phase were also detected.

The obtained results can be interpreted by changes in thermodynamic conditions in the laser-affected zone resulting from vacuumization and multi-stage heating. The absence of oxygen reduces the formation of oxides on the particle surfaces, promoting wettability and diffusion of components. The reduction in pore size and roundness is a consequence of decreased melt viscosity during the remelting stage, which allows surface-tension forces to homogenise the melt more effectively. The formation of a nanograin structure can result from ultra-high cooling rates that limit grain growth. At the same time, the appearance of martensitic 'lamellas' indicates that the concentration of aluminium and nickel in the copper matrix is sufficient to form metastable shape-memory phases directly during the additive synthesis process. The higher intensity of the austenite peaks compared to copper confirms that the combination of pre-heating and vacuum provides the necessary energy balance for dissolving the element powders and forming an intermetallic compound.

The microstructural states observed in Figures 7-10 are intermediate stages of synthesis. Due to the high thermal conductivity of copper, it is possible to obtain a 'structural fingerprint' of the SLM process. Since particle consolidation is incomplete, we can observe diffusion zones at the interfaces between copper, aluminium, and nickel particles. To gain a deeper understanding of particle consolidation, and to study the process of selective laser melting of particles at the atomic level, molecular dynamics simulations were carried out for nanoparticles containing a number of atoms corresponding to the elemental composition of the investigated alloy. To identify the phenomena occurring at the interface between particles, a model with three particles (copper, aluminium, and nickel) was used for the analysis.

Figure 11a illustrates the main stages of melting and diffusion mixing of metal particles. Here, the dark gray atoms represent aluminium, the light gray ones represent nickel, and the orange spheres represent copper. Based on

the results of a visual analysis, we can conclude that mixing begins after the aluminum melts, following its wetting of the copper and nickel. Upon reaching a temperature of 1354 K, the particles became fully mixed, after which we observed homogenization of the melt during further heating.

The process of diffusive mixing of atoms during melting was studied based on the analysis of atomic motion trajectories shown in Figure 11b. As we can see, the formation of a neck between copper and aluminum particles begins with the diffusion of aluminum atoms at a temperature of about 406 K. At a temperature of 822 K, the rate of diffusion mixing increases, due to the higher concentration of vacancies in the neck region between particles and their migration into the particle volume. At the same time, the migration of vacancies toward the center of the particle causes atoms to diffuse toward the neck. The mixing process of aluminum and copper is approaching completion at a temperature of approximately 1354 K (Fig. 11), which is close to the melting point of copper. At this temperature, only a small amount of nickel, which has not diffused remains. To ensure complete homogenization of the melt, the simulation was carried out up to a temperature of 1779 K, which is 50 K higher than the melting point of nickel.

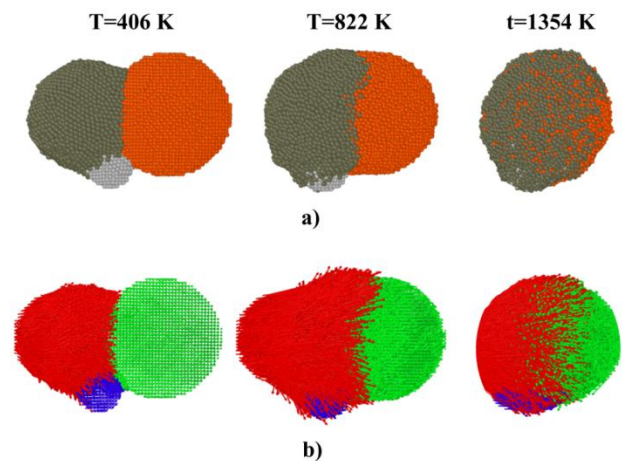


Fig. 11. Visualization of the melting process of copper, aluminum, and nickel particles according to the simulation results

In addition to a study of the mixing process of copper, aluminum, and nickel particles, we analyzed fragments of atomic structures with different types of ordering, corresponding to the nearest neighborhood of atoms in the crystalline state (Fig 12). The Ackland-Jones method was used for this purpose [27]. According to this method, each atom is assigned a crystal structure whose local environment corresponds to one of the known structures (body-centered cubic, face-centered cubic, body-centered hexagonal, or icosahedral). Figure 12 shows the evolution of the percentage of atoms with different neighbor configurations within two temperature ranges that were studied. The first temperature range corresponds to the diffusion mixing of atoms, and the second to homogenization.

It should be noted that all components of the investigated alloy have a face-centered cubic lattice in the

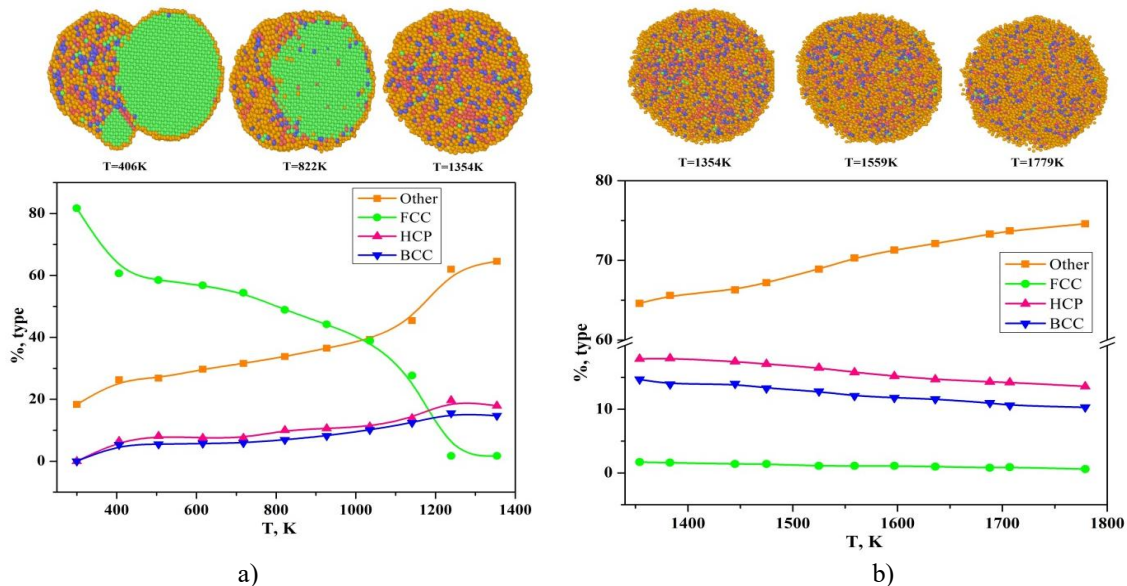


Fig. 12. Evolution of the atomic structure of $\text{Cu}_{81.6}\text{Al}_{14.4}\text{Ni}_4$ alloys during melting of elemental powders

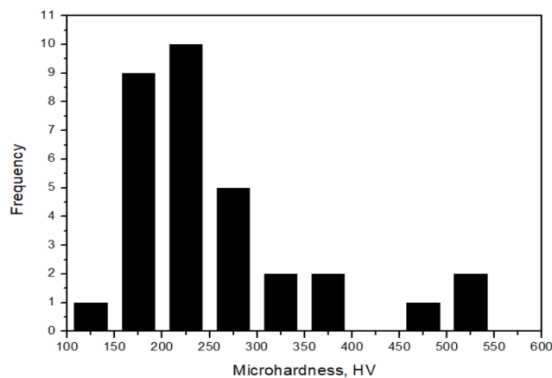


Fig. 13. Vickers microhardness of the alloy synthesized by LPBF

Statistical analysis	
Number of measurements	32
Average value	253 HV
Minimum value	141 HV
Maximum value	518 HV
Arithmetic mean	253 HV
Median	216 HV
Standard deviation	97 HV

crystalline state. Therefore, at the lowest temperature, the fraction of atoms with this type of structure is the highest (Fig 12, a). However, even at the lowest temperature, 20 percent of the atoms belong to structural units with other structure. In this case, the liquid-state structure is marked as other. As the temperature increases, the fraction of atoms corresponding to the face-centered cubic (FCC) structure decreases, while the amount of the liquid phase increases. At a temperature of 1354 K, the number of atoms with a FCC structure approaches zero. Despite this, the resulting nanoparticle exhibits elements of structure with an ordering similar to that of body-centered cubic (BCC) and hexagonal close-packed (HCP) lattices. Given that the structure of the FCC lattice, in terms of its nearest packing, is similar to that of the HCP structure, we can assume that the formation of the latter is the result of a slight FCC-HCP transformation.

It is important to note that the structure with the nearest neighborhood of atoms which corresponds to the body-centered cubic lattice is formed during melting. This structure can form as a result of the decrease in atomic packing density that occurs during heating. The maximum amount of atoms with this configuration is about 15 percent at a temperature of 1354 K. An increase in temperature leads to a decrease in the fraction of atoms with a body-centered cubic structure and to an increase in

the percentage of atoms with a structure typical of a melt. Based on the obtained results of the formation of the structure in the liquid state, we can assume that during crystallization of the alloy, regions with a body-centered cubic (BCC) structure may serve as crystallization centers for the phases, leading to the formation of a similar structure in the crystalline state.

X-ray analysis and microstructure studies indicated the formation of a composite with a multiphase structure consisting of local regions of pure copper and Cu-Al-Ni alloy. To investigate the mechanical properties of the material directly within the consolidated zones, microhardness measurements were performed by the Vickers method. This approach allowed us to avoid the influence of pores or macrodefects and to determine the local resistance of the synthesized material to plastic deformation, which is important for understanding the functional characteristics of the alloy.

The total averaged value of the microhardness of the studied sample was 253 HV. Fig 13 shows the frequency distribution of HV values over the sample and its statistical analysis. A standard deviation is very high (of about 40% of the mean value) indicating that the material is not homogeneous. The value of 518 HV indicates the presence of very hard local areas, which may be intermetallic inclusions or martensitic grains with a high

density of lattice defects. The frequency distribution is asymmetric. Most values are grouped within 150 – 250 HV. For comparative analysis the microhardness is 100–150 HV for Cuprum, 150–200 HV for Austenite, and 200 – 350 HV for Martensite.

However, it is worth noting that the overall microhardness for a composite material is not enough informative. Given the structural heterogeneity of the samples, a local-averaged sampling strategy was employed. Microhardness measurements were performed within condensed fragments ('islands') of the metal matrix that remained after mechanical polishing of the sample. A series of 5-7 imprints were performed for each 'island', and then they were averaged to obtain a representative value of local microhardness (site-specific microhardness assessment). Therefore, Table 2 shows 'region-specific' local microhardness values. Since microhardness is structure-sensitive, significant deviations in local values are most likely due to differences in phase composition and the degree of consolidation of powder particles. Such dispersion in mechanical properties also correlates with XRD results, confirming the phase heterogeneity of the alloy, which is inherent for incomplete homogenization of the components during LPBF synthesis.

Table 2.

Site-specific microhardness measurements	
Average microhardness, HV	Local microhardness, HV
253.4 ± 80.2	260,80 ± 26,6
	339,11 ± 40,4
	195,77 ± 28,7
	156,4 ± 11,9
	346,54 ± 142,9
	209,51 ± 20,5

Conclusions

The paper analyzes the microstructure and mechanical properties of Cu-Al-Ni alloys synthesized by the LPBF method using a mixture of metal powders. The transient

morphological states of the samples were investigated which can be considered as informative model structures that allow us to investigate the evolution of the material from a mechanical mixture of powders to a functional intermetallic alloy, which is important for understanding the physics of the formation of shape memory phases in additive manufacturing. The formation of a heterogeneous multiphase structure with nanostructuring (grain sizes < 50 nm) was detected, which is a consequence of high cooling rates and temperature gradients inherent in the SLM process.

Analysis of the X-ray diffraction curves of the sample obtained under optimized SLM modes demonstrated a significant evolution of the phase composition. It was found that the intensity of the main austenite reflex is twice as high as the intensity of the residual copper peak Cu. This indicates that the selected laser scanning parameters provided sufficient thermal load for deep alloying of the powder mixture components. The dominance of the austenite phase in combination with the submicron cellular structure confirms the formation of a functional alloy with the shape memory phases.

Computer simulations demonstrate that, under the laser processing conditions used in this study, austenitic phase nuclei can form directly from the liquid state. This is supported by the formation of micro-regions with a BCC-type structure immediately after melting and their existence over a wide temperature range.

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Синтез композитів із пам'яттю форми методом лазерного спікання порошку

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У цій роботі досліджується вплив різних параметрів лазерної обробки, а також атмосфери на еволюцію мікроструктури порошкового сплаву Cu-Al-Ni та утворення фаз з пам'яттю форми, синтезованих за допомогою лазерного спікання порошкової суміші чистих елементів методами селективного лазерного спікання/плавлення (selective laser sintering/melting, SLS, SLM). Експериментальні результати показали, що синтез у вакуумі 10^{-2} Па замість атмосфери повітря значно покращує консолідацію частинок порошку, запобігаючи утворенню оксидів. Методами X-променевого дифракційного аналізу та сканувальної електронної мікроскопії досліджено, що в результаті багатостадійного лазерного сканування, що включає попереднє нагрівання та постобробку, утворюється гетерогенна мікроструктура, що включає аустенітну та мартенситну фази, які відповідають за ефект пам'яті форми. Аналіз кривих рентгенівської дифракції зразка, отриманого в оптимізованих режимах SLM, показує складну еволюцію фазового складу. Було виявлено, що інтенсивність основного аустенітного рефлексу вдвічі вища, ніж інтенсивність залишкового піку міді Cu. Це свідчить про те, що вибрані параметри лазерного сканування забезпечили достатнє термічне навантаження для глибокого легування компонентів порошкової суміші. Завдяки високим швидкостям охолодження вдалося зафіксувати перехідні морфологічні стани зразків, які можна розглядати як інформативні модельні структури, що дозволяють дослідити еволюцію матеріалу від порошкової суміші до функціонального градієнтного композиту, що важливо для розуміння фізики формування фаз з пам'яттю форми в адитивному виробництві. Комп'ютерне моделювання проведене методом молекулярної динаміки, демонструє, що за умов лазерної обробки, що використовуються в цьому дослідженні, зародки аустенітної фази можуть формуватися безпосередньо з рідкого стану. Це підтверджується утворенням мікрообластей зі структурою типу ОЦК одразу після плавлення та їх існуванням у широкому діапазоні температур. Результати дослідження мікротвердості показують значну варіативність значень локальної мікротвердості, що пояснюється складною гетерогенною композитною структурою. Домінування аустенітної фази в поєднанні з субмікронною комірчастою структурою підтверджує формування функціонального сплаву з фазами з ефектом пам'яті форми.

Ключові слова: сплав Cu-Al-Ni, сплав з пам'яттю форми, адитивне виробництво, селективне лазерне плавлення, лазерне спікання порошку на підкладці, мікротвердість, функціональний градієнтний композит.