

Article

Modelling Crystalline α -Mg Phase Growth in an Amorphous Alloy $\text{Mg}_{72}\text{Zn}_{28}$

Bartosz Opitek ^{1,*}, Paweł L. Żak ^{1,*} , Janusz Lelito ^{1,*}  and Vincent Vignal ²

¹ Faculty of Foundry Engineering, AGH University of Krakow, 23 Reymonta Street, 30-059 Cracow, Poland; bartek3185@wp.pl

² ICB, UMR 6303 CNRS, Université de Bourgogne, BP 47870, Cedex, 21078 Dijon, France; vincent.vignal@u-bourgogne.fr

* Correspondence: pawelzak@agh.edu.pl (P.L.Ż.); lelito@agh.edu.pl (J.L.)

Abstract: A model of α -Mg grain growth in an amorphous $\text{Mg}_{72}\text{Zn}_{28}$ alloy matrix was developed together with numerical software. Its application enables tracking the growth process of the α -Mg phase in an amorphous alloy. The model was based on the diffusion-driven growth of α -Mg in an amorphous alloy under appropriate boundary conditions at an isothermal annealing temperature and taking into account the presence of a grain with an initial radius of 1 nm. The numerical model was based on a mathematical model of heat flow, described by the Fourier–Kirchhoff equation, and diffusion, described by Fick’s second law. The initial boundary conditions necessary to simulate grain growth in the amorphous phase were established. The results of the numerical simulation indicate grain growth with increasing isothermal annealing temperature and increasing isothermal annealing time.

Keywords: amorphous structure; crystallisation; $\text{Mg}_{72}\text{Zn}_{28}$ alloy; numerical methods; metallic glass



Citation: Opitek, B.; Żak, P.L.; Lelito, J.; Vignal V. Modelling Crystalline α -Mg Phase Growth in an Amorphous Alloy $\text{Mg}_{72}\text{Zn}_{28}$. *Appl. Sci.* **2024**, *14*, 3008. <https://doi.org/10.3390/app14073008>

Academic Editor: Manoj Gupta

Received: 24 February 2024

Revised: 28 March 2024

Accepted: 30 March 2024

Published: 3 April 2024



Copyright: © 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

1. Introduction

Computer simulations are used to describe various phenomena that occur during the crystallisation process. The development of knowledge and technology, which has been progressing for several decades, allows for the continuous improvement of the tools used, especially at the level of numerical calculations. More and more modern computational methods are used, which yield more satisfactory results and, more importantly, are very often consistent with the actual behaviour of the simulated materials [1].

In recent years, numerical models have been used to study nucleation and grain growth processes during the crystallisation of metallic glasses [2]. Stefanescu [3] proposed a division into macroscopic models (first generation) and micro-/macro-models (second generation). First-generation models are based on the relationship between the proportion of the locally solidified phase and temperature. Second-generation models are characterised by the inclusion of the laws of nucleation and grain growth in the calculations, which is typical for modelling at the micro-level [4].

The first work related to modelling the nucleation and growth of grains in alloys with an amorphous structure (called metallic glasses) was carried out by Uhlmann [5]. He derived equations that combine classical theories of nucleation and growth and those taken from the Kolmogorov–Johnson–Mehl–Avrami theory. This allowed for the determination of time–temperature transition diagrams and the prediction of critical cooling rates for various metallic glasses. Morris [6] modelled crystallisation in the Ni–Si–B system. In this case, the author combined the thermodynamic model by Thompson and Spaepen [7] with the previously mentioned Uhlmann model. Gránásy [8], in turn, used the Gibbs free energy for his model. He calculated the crystallisation kinetics for the $\text{Fe}_{40}\text{Ni}_{40}\text{P}_{14}\text{B}_6$ metallic glass by measuring the difference in specific heat between the liquid and crystalline phases.

Ge et al. [9] used the Uhlmann and CALPHAD kinetics databases, which allowed for the prediction of the possibility of obtaining metallic glasses of Cu-Zr and Cu-Zr-Ti.

All the works cited above, as well as others [10–13], assume polymorphic conditions, which means an equal chemical composition of the particle and matrix phases. Crystallisation then depends on the rate of attachment of atoms at the phase boundary, while the coupling related to grain growth and transport through diffusion to the grain-matrix phase boundary is omitted. Suryanarayana et al. [14] and Köster et al. [15] showed that polymorphic crystallisation is quite rare in metallic glasses.

A model that fully shows the kinetics of the crystallisation of metallic glasses should describe both the nucleation of crystals and the growth of grains controlled by the diffusion and dissolution of particles. Such a model should show the phase transition under both isothermal and non-isothermal conditions. It is possible to design a numerical simulation model that, using appropriate models of the nucleation and growth division in metallic glasses, shows the evolution of the crystal size distribution over time.

The modelling of the nucleation, growth, and dissolution of crystals for the amorphous Al-Cu-Zr alloy was shown by Ericsson et al. [2]. In this model, the authors used two theories: the classical nucleation theory and the diffusion-controlled multicomponent growth developed by Chen [16]. This method was then implemented using the numerical scheme of Kampmann and Wagner [17], which was designed by Myhr and Grong [18]. In a recent publication, it was noted that the concentration gradient causes the movement of atoms, which are excited by high temperatures, causing a largely diffusive phase transformation [19,20]. Due to the increase in temperature, secondary reactions occur. If they are formed from a supersaturated solid solution, three important processes occur [17,21,22]: nucleation, growth, and thickening. The first two processes are driven by the change in the free energy of the transformation and end when the equilibrium volume fraction of the resulting phase is reached. Grain coarsening, on the other hand, is driven only by a reduction in surface energy and continues until a particle emerges. The presented model used the works of Kampmann et al. [17,22] and Langer and Schwartz [23], where the three processes mentioned above were incorporated into the numerical simulation. An appropriate model (i.e., one that can handle rapid temperature fluctuations) should include a control volume-based flux balance formulation [24].

The model by Myhr and Grong [18] comprises three important elements: (i) the nucleation model, which predicts the number of stable nuclei at each computational time step; (ii) the rate law, which calculates the rate of dissolution or growth for each discrete particle size class; and (iii) the continuity equation, which records the amount of solute in precipitates. In the model by Ericsson et al. [2], the model by Myhr and Grong [18] was coupled with the CALPHAD database of the Al-Cu-Zr system [24], and the following assumptions were made: (i) spherical shape of grains with a sharp boundary between the grains and the matrix; (ii) cross-diffusion of elements is neglected, while the diffusion of alloying elements in the matrix is equal; (iii) nucleation takes place at a fixed rate; (iv) a local equilibrium corrected by the Gibbs–Thomson effect is maintained at the grain-matrix boundary; (v) molar volumes of the grain and matrix are assumed to be equal; and (vi) grain growth is fully controlled by diffusion in the matrix. All these assumptions made it possible to assess the thermodynamic properties dependent on the phase-transition temperature and chemical composition of the amorphous glass. In addition, they considered the imperfect mixing present in all such materials. The numerical model was built based on a comparison of time–temperature diagrams of the transformation and continuous heating/cooling transformation. The formation of intermetallic phases was simulated under isothermal and non-isothermal conditions. The results obtained were consistent with the experimental data, confirming the correctness of the selected model.

Numerical modelling shows great potential for predicting crystallisation in the case of amorphous alloys. The great advantage of simulations of this type is their low cost, along with other advantages including the ability to perform them under almost any condition, revealing many previously unforeseen defects in the material, or even avoiding unnecessary

attempts at costly production of a previously designed material. Some amorphous alloys crystallise after a very long time, and numerical models will now allow for checking many different properties of them [25].

2. Materials and Experimental Results

First, a mathematical model of grain growth was developed based on the diffusion model described in the next section. Using this model, several numerical calculations were performed. The results of these calculations (grain size) were compared with the results obtained from the experiment. For this purpose, a two-component eutectic alloy $\text{Mg}_{72}\text{Zn}_{28}$ was produced by casting in a resistance furnace under the protection of argon as an inert gas. Both magnesium and zinc were 99.9% pure. Liquid $\text{Mg}_{72}\text{Zn}_{28}$ alloy was poured into the steel mould cavity. In this way, a cylindrical sample with a diameter of 20 mm and a height of 50 mm was obtained. Then, this sample was rolled to a diameter of 10 mm. The sample was melted using a melt-spinning device to cast a ribbon with an amorphous structure. The thickness of the obtained ribbon was 150 μm , and the peripheral speed of the wheel was 40 m s^{-1} . Both processes, i.e., melting and casting, took place under the protection of argon as an inert gas. The obtained ribbons were subjected to X-ray diffraction tests to confirm the amorphous structure. The X-ray diffraction (XRD) results were collected using a Panalytical Empyrean diffractometer (Almelo, Nederland) equipped with a $\text{Cu K}\alpha$ X-ray source. The next step was to verify the simulation results with an experiment. For this purpose, the amorphous ribbons were subjected to isothermal annealing heat treatment at selected temperatures. Heat treatment was carried out with high-purity argon using a TA DSC Q20 differential scanning calorimeter (Eschborn, Germany). The rate of heating the amorphous ribbon to the isothermal annealing temperature was 80 K min^{-1} . The ribbon was held at an isothermal annealing temperature for 300 s and then cooled to ambient temperature at a rate of 80 K min^{-1} . Grain size tests were performed using a JEOL JSM-7600F field emission scanning electron microscope (FE-SEM).

3. Mathematical Model and Calculation Results

The presented model concerns the crystallisation of the two-component amorphous alloy $\text{Mg}_{72}\text{Zn}_{28}$. This study analysed the increase in the primary phase of α -Mg. In this work, the presented model concerns the analysis of the grain growth rate in the amorphous phase as a function of the isothermal annealing temperature. Therefore, certain assumptions are necessary to perform the correct numerical calculations.

The binary $\text{Mg}_{72}\text{Zn}_{28}$ alloy faces difficulty in obtaining an amorphous structure. This is due to the small amount of alloying elements. As widely known, multicomponent alloys, where the atomic sizes of individual alloy components differ by approximately 20%, have a better tendency towards glass transition (containing an amorphous structure). Therefore, attempts were made to select a chemical composition as close as possible to the eutectic one, as shown in the phase equilibrium system of the Mg-Zn alloy (blue line) in Figure 1. This chemical composition facilitates the production of an amorphous alloy as a result of the small range between the liquidus temperature and the solidus. Line number 1 is an extension of the liquidus line, determined using the formula $y = -0.0077x + 5.0323$. Line number 2 is an extension of the solidus line, determined using the formula $y = -0.0002x^2 + 0.0637x + 24.462$. The red line indicates one of the isothermal temperatures at which numerical calculations can be performed.

The crystallisation kinetics simulation shows grain growth in the amorphous phase. Therefore, it is assumed that the seed exists from the very beginning as a ball and grows. The initial grain radius assumed for the calculations is 1 nm, while the end of the calculations is determined by the simulation time. The simulation takes place within a fixed domain with a radius of 200 nm. The scheme used for this calculation model is shown in Figure 2, which additionally indicates how the zinc (Zn) concentration will change.

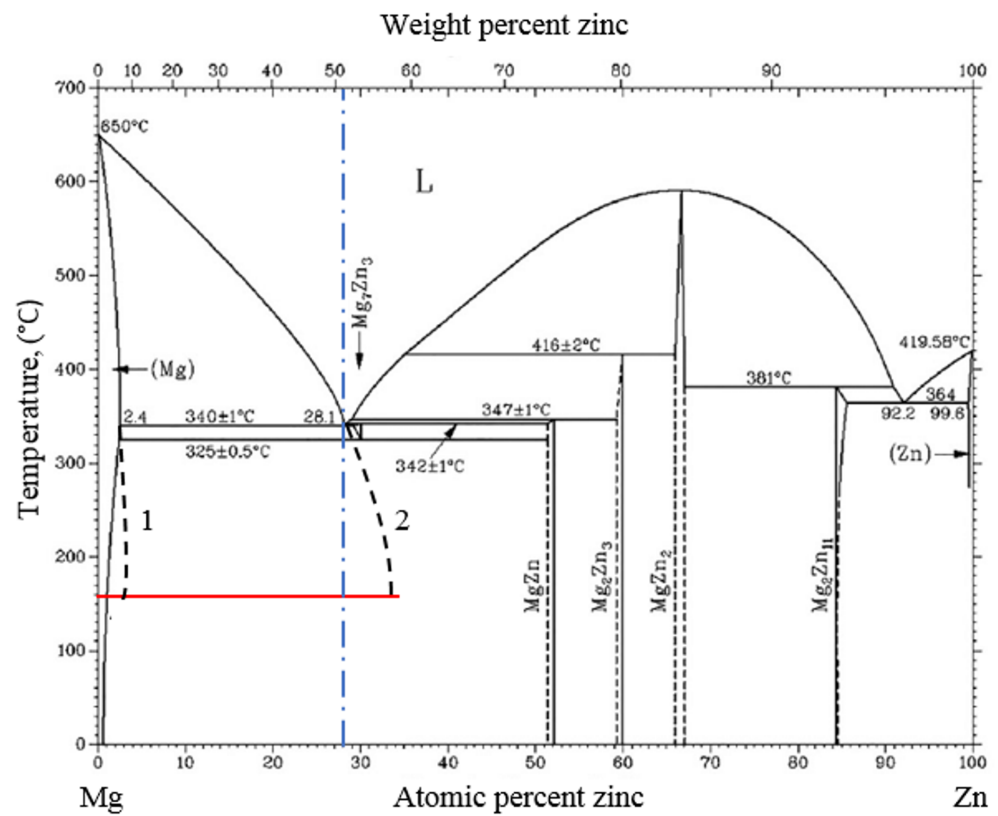


Figure 1. Mg-Zn phase equilibrium system.

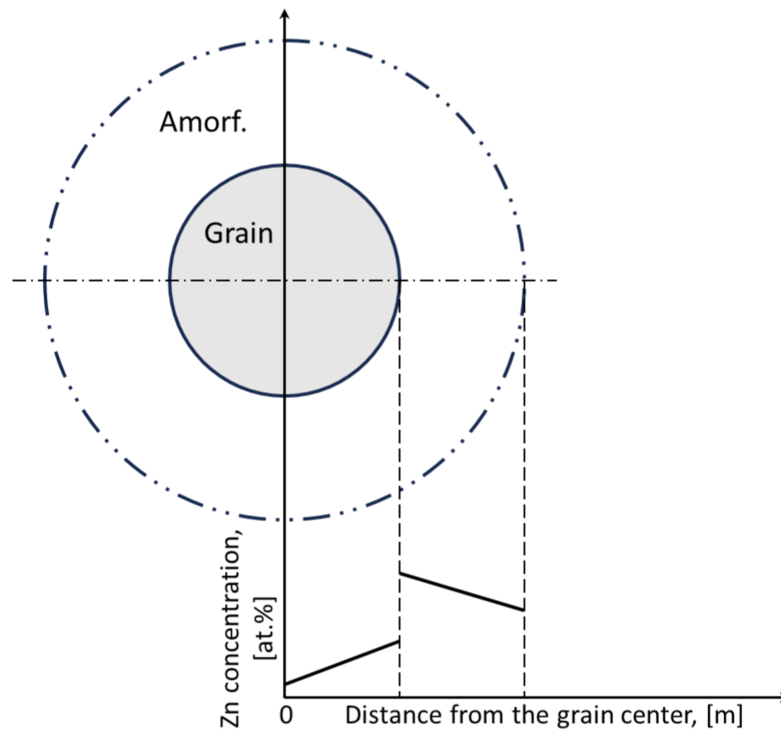


Figure 2. Diagram of grain growth and zinc concentration distribution in the grain and the amorphous phase.

The numerical model used in the simulation used the Fourier–Kirchhoff equation [26], which is one of the simplest solutions for this type of simulation. It describes the heat flow

in solidifying casting, but it can also be used for research on amorphous alloys, where the Fourier–Kirchhoff equation allows for calculating how heat flows in the material. This is macro-level modelling that ignores more detailed micro-level assumptions. The model used in this work included certain simplifications (this allowed us to largely simplify the complexity of the calculations and, consequently, the durations of their execution), such as the omission of the internal heat source and the assumption of constant thermophysical parameters. The calculations were performed in a one-dimensional system. The Fourier–Kirchhoff equation used in this work to calculate the numerical model has the form:

$$c_v \cdot \frac{\partial T}{\partial \tau} + c_v \cdot u \cdot \text{grad}T = \text{div}(\lambda \cdot \text{grad}T) + q_v, \quad (1)$$

where c_v is the volumetric-specific heat ($\text{J} \cdot \text{m}^{-3} \cdot \text{K}^{-1}$), T is the temperature (K), τ is the time (s), λ is the thermal conductivity ($\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$), u is the velocity vector ($\text{m} \cdot \text{s}^{-1}$), and q_v is the solidification-related heat source function ($\text{W} \cdot \text{m}^{-3}$).

Numerical calculations were performed on the amorphous $\text{Mg}_{72}\text{Zn}_{28}$ alloy, assuming that the growth control process would be diffusion. The grain, which exists from the very beginning, has a surface that separates it from the remaining volume in the form of an amorphous phase. The grain surface changes with the progressive crystallisation of $\text{Mg}_{72}\text{Zn}_{28}$; therefore, this change is described by Fick's second law [27] related to diffusion. It takes the following form characterised by a constant value of the diffusion coefficient in a spherical system:

$$\frac{\partial C(l, \tau)}{\partial \tau} = D \cdot \left(\frac{\partial^2 C(l, \tau)}{\partial l^2} + \frac{2}{l} \frac{\partial C(l, \tau)}{\partial l} \right), \quad (2)$$

where C denotes the concentration of the element (mass%), l denotes the distance from the grain centre (m), and D denotes the diffusion coefficient of the element ($\text{m}^2 \cdot \text{s}^{-1}$).

The change in zinc concentration in the growing grain is shown in Figure 3. The concentration of zinc in the grain is denoted as C_{grain} . The concentration of zinc at the phase boundary on the grain side is denoted as $C_{\text{grain/amorph}}$, while on the amorphous side, it is denoted as $C_{\text{amorph/grain}}$. The concentration of zinc in the amorphous phase is denoted as C_{amorph} . The growth of the grain in the numerical simulation takes place in time steps, which are denoted as k in the diagram. After one time step (k), the grain has grown by a unit of length denoted as dl in the diagram. Meanwhile, the concentrations at the phase boundary change. The initial assumption is that the zinc concentration in the grain (C_{grain}) is 0%, and in the amorphous phase (C_{amorph}), it is 28%.

The calculations performed in the simulation used a finite-volume numerical method. This method was selected for its speed and ease of implementation for the amorphous $\text{Mg}_{72}\text{Zn}_{28}$ alloy. The equations of Fick's second law describing the concentration change in the grain are given by the following equation:

$$\frac{\partial C_{\text{grain}}}{\partial \tau} = D_{\text{grain}} \cdot \left(\frac{\partial^2 C_{\text{grain}}}{\partial l^2} + \frac{2}{l} \frac{\partial C_{\text{grain}}}{\partial l} \right), \quad (3)$$

and in the amorphous phase,

$$\frac{\partial C_{\text{amorph}}}{\partial \tau} = D_{\text{amorph}} \cdot \left(\frac{\partial^2 C_{\text{amorph}}}{\partial l^2} + \frac{2}{l} \frac{\partial C_{\text{amorph}}}{\partial l} \right), \quad (4)$$

and at the phase boundary, X_k , the mass balance equation is introduced [28]:

$$\left(C_{\text{grain/amorph}}^* - C_{\text{amorph/grain}}^* \right) \frac{dl}{d\tau} = D_{\text{amorph}} \left(\frac{\partial C_{\text{amorph}}}{\partial l} \right)_{X_k^+} - D_{\text{grain}} \left(\frac{\partial C_{\text{grain}}}{\partial l} \right)_{X_k^-}. \quad (5)$$

The zinc diffusion coefficient in the grain of the primary magnesium phase is equal to $D_{\text{grain}} = 2.67 \cdot 10^{-4}$, $\text{m}^2 \cdot \text{s}^{-1}$, and in the amorphous phase, $D_{\text{amorf}} = 2.67 \cdot 10^{-3}$, $\text{m}^2 \cdot \text{s}^{-1}$ [29].

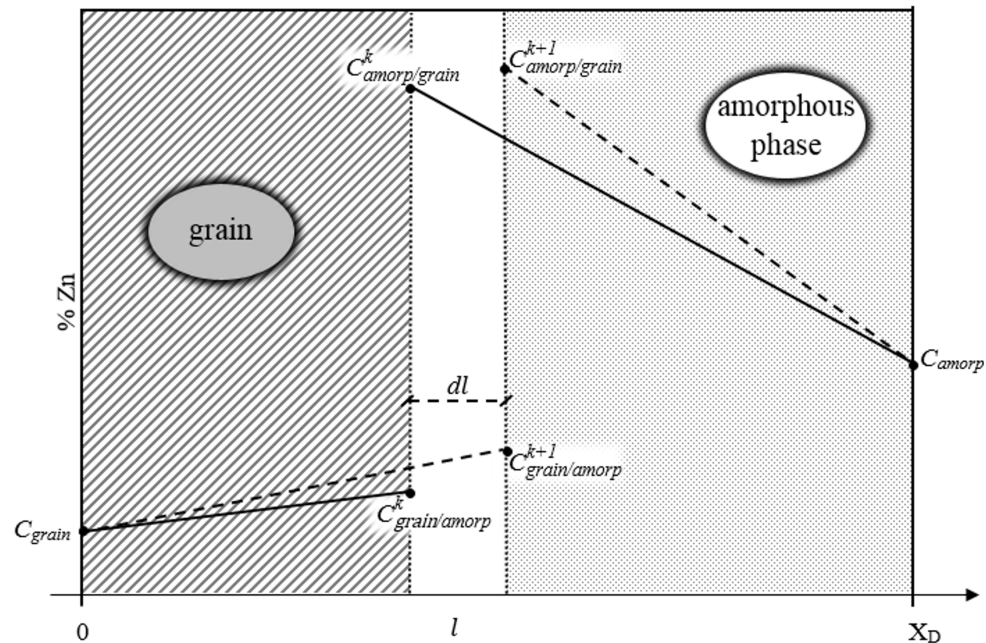


Figure 3. Scheme showing how the concentration changes in the grain/amorphous matrix system.

The following boundary conditions were adopted for the calculations:

- In the grain centre, $l = 0$, $\rightarrow \frac{\partial C_{\text{grain}}}{\partial l} = 0$;
- In the amorphous phase, *very far* from the growing grain, $l = X_D$, $\rightarrow$ the constant concentration value equal to the initial concentration C_0 (Dirichlet boundary condition);
- At the phase boundary, the concentrations were calculated using Equation (5), and

$$\int_0^{X_k} C_{\text{grain}} dl + \int_{X_k}^{X_D} C_{\text{amorf}} dl = \int_{l_0}^{X_d} C_0 dl, \quad (6)$$

where l_0 is the initial grain size.

4. Results of Numerical Simulation

The numerical simulation showing grain growth in the amorphous phase of the $\text{Mg}_{72}\text{Zn}_{28}$ alloy required additional assumptions. Appropriate isothermal annealing temperature values were necessary. Based on the research carried out in the work of Opitek et al. [30] for the amorphous $\text{Mg}_{72}\text{Zn}_{28}$ alloy, the following values were selected: 350 K, 352 K, 353 K, 353.5 K, and 354 K. The total crystallisation time for each of these temperature values was, respectively, 6001 s, 4067 s, 2916 s, 2644 s, and 2447 s. The simulation results are shown in Figure 6. Each graph shows the increase in grain size in the amorphous phase over time for a given isothermal annealing temperature. At the same time, the diffusion of zinc into the grain continued. Therefore, the concentration of this element in the grain increased. It can also be seen how the crystallisation front shifted with the progressing phase transformation. Zinc accumulated at the phase boundary and was displaced by the crystallisation front moving over time. This was mainly due to the inability to diffuse so much zinc into the growing grain.

At an isothermal annealing temperature of 354 K, the grain size increased from 20 nm after 50 s to 70 nm after 300 s of isothermal annealing.

The ribbon produced from the binary $\text{Mg}_{72}\text{Zn}_{28}$ alloy was examined using XRD. The results of these tests are presented in Figure 4. In the plot, only the background is visible,

represented by the presence of the so-called amorphous “halo” with no local peaks. The X-ray diffraction pattern is characterised by a high level of background “noise” in relation to the maximum intensity. These observations of the XRD results of the ribbon allow us to identify its amorphous character. The amorphous ribbon of the binary $\text{Mg}_{72}\text{Zn}_{28}$ alloy, after heat treatment and isothermal annealing at a temperature of 354 K for 300 s, was subjected to SEM examination. The results of these tests are presented in Figure 5.

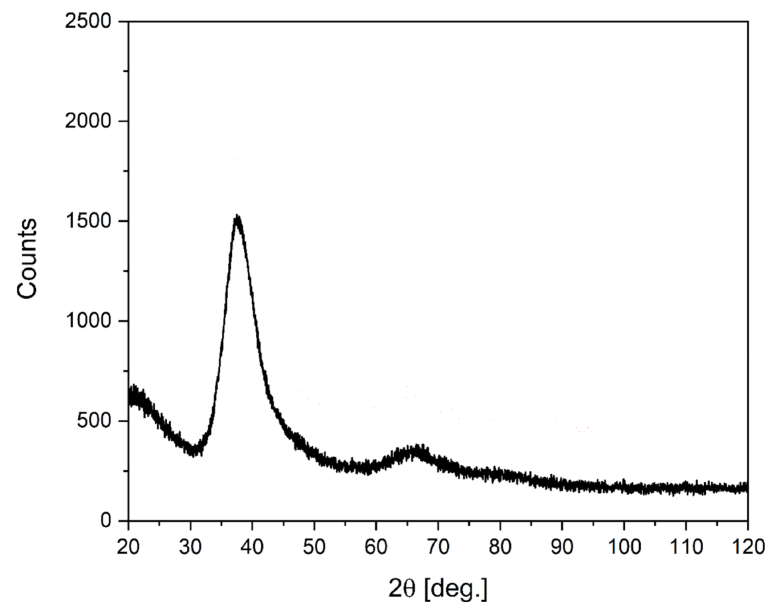


Figure 4. X-ray diffraction patterns of a $\text{Mg}_{72}\text{Zn}_{28}$ cast ribbon.

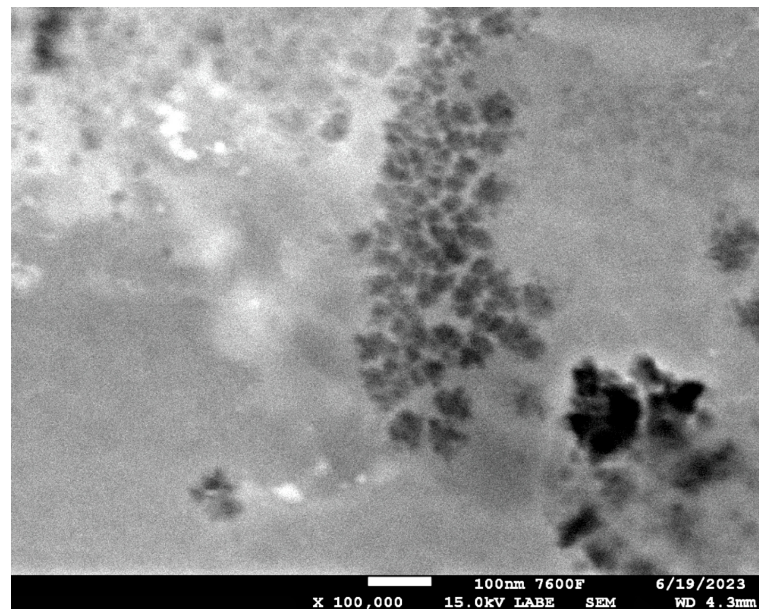


Figure 5. Results of SEM examination of the microstructure of an amorphous ribbon after heat treatment of isothermal annealing at a temperature of 354 K for 300 s.

The average grain size was determined using the secant method. The average grain size was approximately 71 nm.

Figure 6 shows the results of the numerical simulation showing the impact of the annealing temperature on grain growth. The plots display the zinc concentration in the grain and the amorphous phase on the axis, indicating the distance from the grain centre. Different colours correspond to different annealing times: 50, 100, 150, 200, 250, and 300 s. It

can be seen that both the annealing temperature and time affected the grain growth rate and zinc concentration across the whole domain. The key observation is that as the annealing temperature increased, the grain size during the corresponding annealing time also increased. Moreover, the grain size changed more linearly with increasing annealing temperature compared to lower annealing temperatures. The character of the zinc concentration for each annealing time in the grain did not differ significantly at its radius. The zinc concentration in the whole grain was more or less the same. However, as the grain increased or the annealing time increased, the zinc concentration in the grain also increased. This may have been caused by the zinc diffusion through the grain boundary from its reach regions in the amorphous phase. The characteristics of the zinc concentration in the grain did not show any clear functional trend. In the amorphous phase, even for longer annealing times, a higher zinc concentration in the grain was observed; near the grain boundary, a higher zinc concentration was also observed. The zinc concentration in the amorphous phase was highest at the grain boundary in all the cases analysed. As the distance from the grain boundary increased, the concentration of zinc in the amorphous phase decreased. At the end of the computational domain, the zinc concentrations were almost identical. With increasing annealing temperature, the increase in the zinc concentration in both the grain and the amorphous phase near the grain boundary was observed. At higher annealing temperatures, faster grain growth was observed. At a higher growth rate, the remaining elements in the amorphous phase were pushed by the grain, causing an increase in their concentrations in the phase that surrounded the grain. The diffusion rates in the crystalline and amorphous phases remained constant, resulting in a higher element concentration at the grain boundary because grain growth was faster. It is worth mentioning that mass conservation was ensured during each simulation. Additionally, as the annealing temperature increased, an increase in zinc concentration in the grain was observed. This phenomenon was even more visible for longer annealing times. At an annealing temperature of 350 K and an annealing time of 300 s, the zinc concentration in the grain was approximately 3.52 wt.%, and at an annealing temperature of 354 K and an annealing time of 300 s, it was about 3.58 wt.%. A similar trend was observed for the amorphous phase near the grain boundary. At an annealing temperature of 350 K and an annealing time of 300 s, the zinc concentration was about 28.6 wt.%, and at an annealing temperature of 354 K and an annealing time of 300 s, the zinc concentration near the grain boundary reached almost 29.4 wt.%.

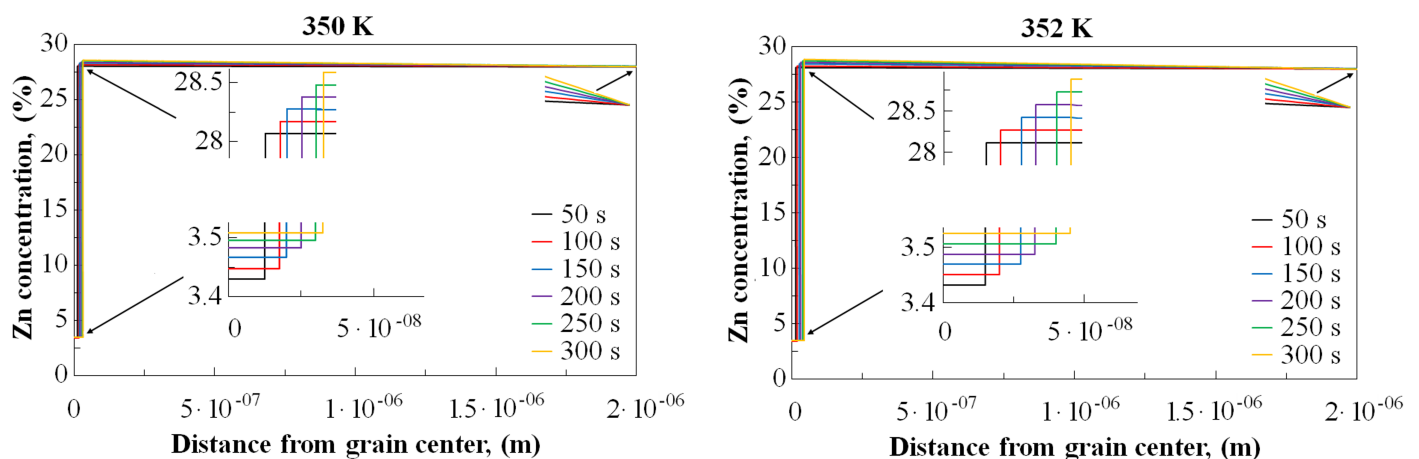


Figure 6. Cont.

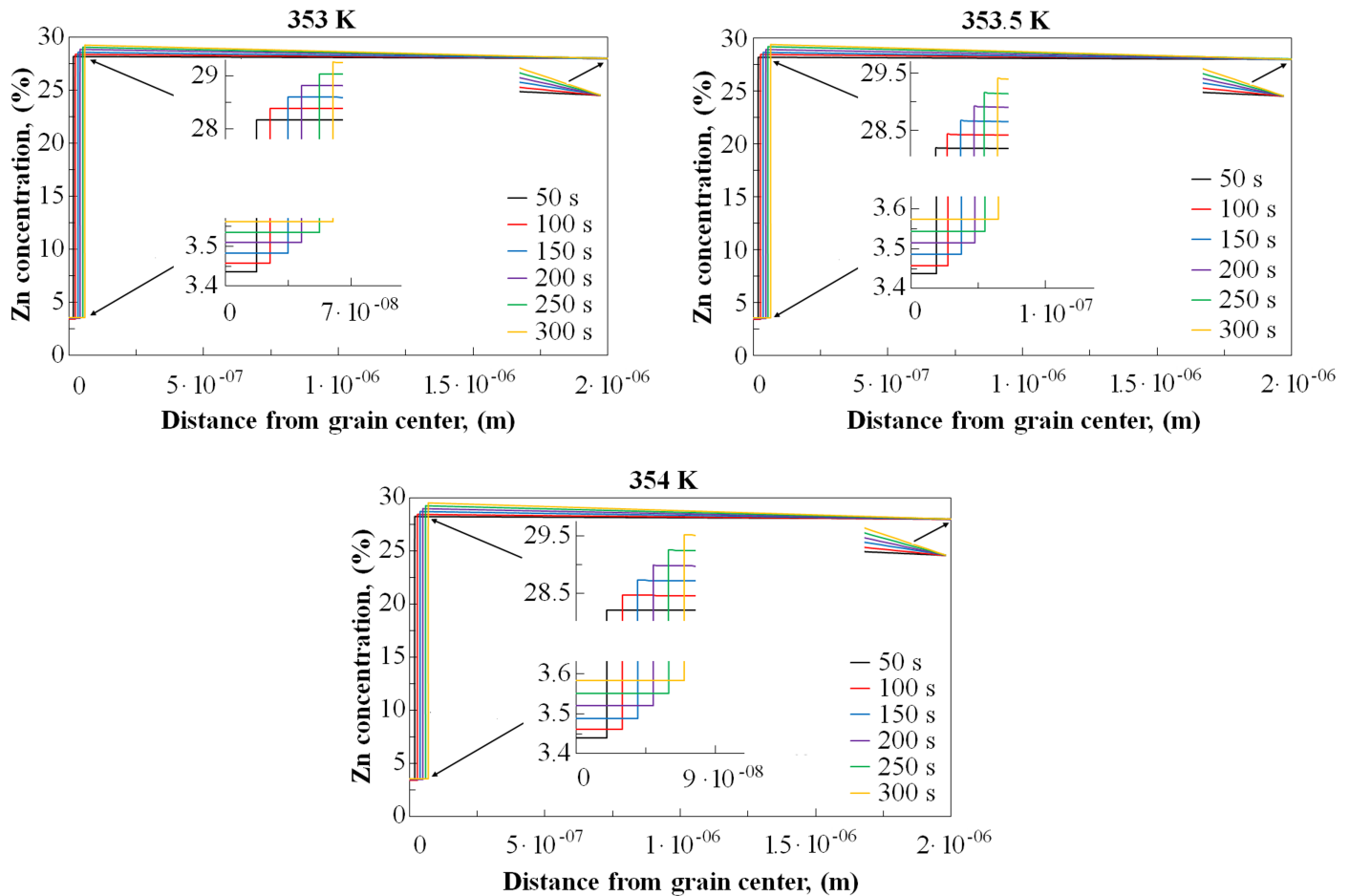


Figure 6. Simulation results of grain growth over annealing time at chosen isothermal annealing temperature values: $T = 350$ K, $T = 352$ K, $T = 353$ K, $T = 353.5$ K, and $T = 354$ K.

The results of the numerical simulation in Figure 7 show the extent of grain growth in the amorphous phase at various temperature values, with time values ranging from 50 s to 300 s, changing every 50 s. The grain grew the fastest at the highest isothermal annealing temperature of 354 K and the slowest at the lowest isothermal annealing temperature of 350 K. Therefore, it can be concluded that as the value of the isothermal annealing temperature decreased, the grain growth rate also decreased. This phenomenon is related to the fact that the diffusion process, which depends on the temperature value, plays a decisive role during grain growth.

Figure 7 depicts the results of the numerical simulation, showing the influence of annealing temperature on the grain growth rate and the zinc concentration within the computational domain. After the given annealing times, grains of different radii were obtained. Across all annealing times, the largest grains were obtained at an annealing temperature of 354 K, whereas the smallest grains were obtained at 350 K. Taking all of the presented results into account, it can be stated that higher annealing temperatures yield larger grains. Similarly, as shown in Figure 6, for larger grains, more zinc was present in the grains. Also, for longer annealing times, the zinc concentration in the grain was higher. The same was observed for the zinc concentration near the grain boundary. For longer annealing times, more zinc was pushed off the added grain volume, and the zinc concentration near the grain boundary increased. The subsequent diffusion within the amorphous phase distributed this element throughout the subdomain; however, this phenomenon was not fast enough to avoid Zn accumulation at the grain boundary region. At maximum, it could be greater than 29 wt.% after 300 s of annealing.

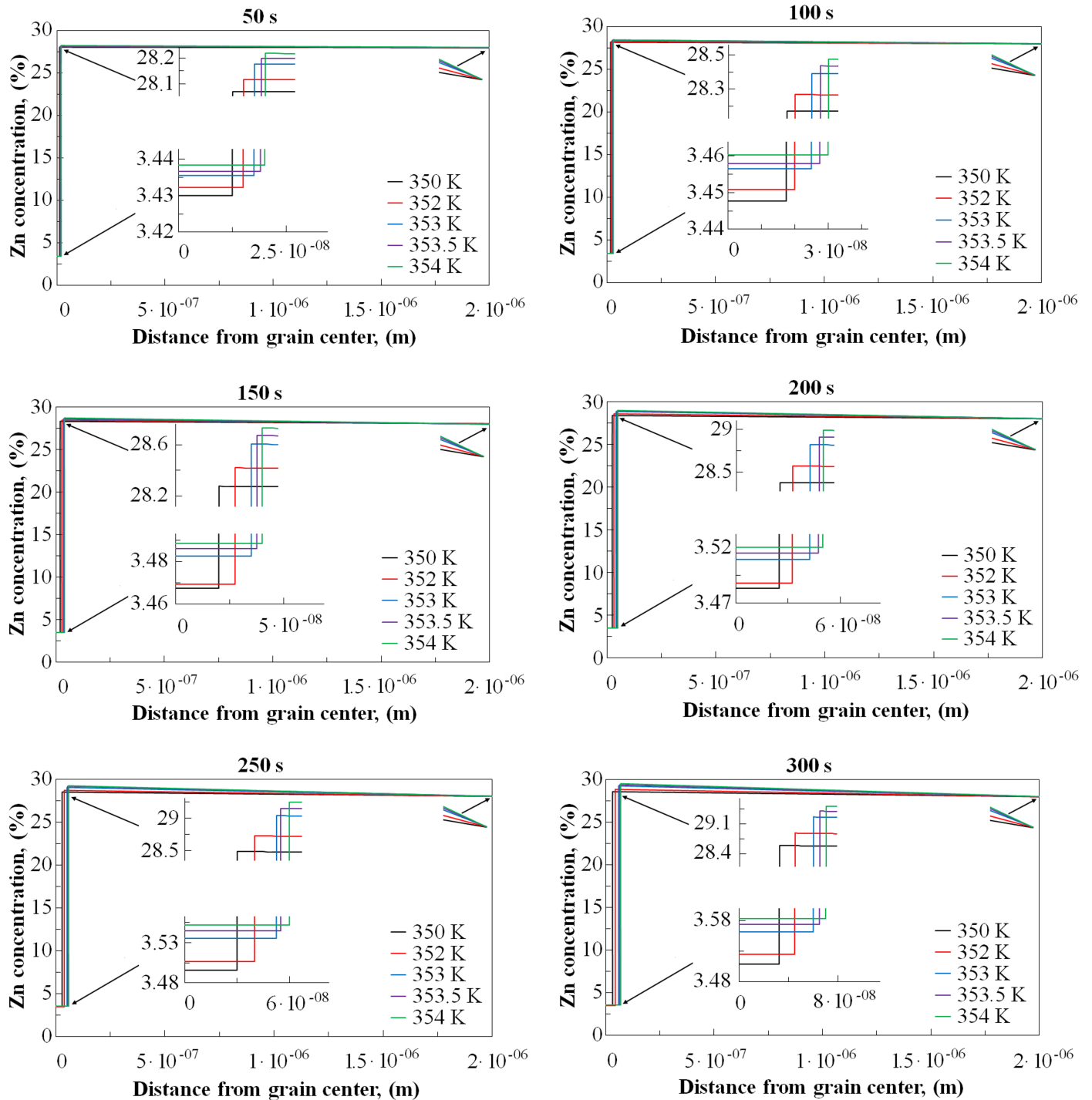


Figure 7. Simulation results of grain growth at various isothermal heating temperatures after selected annealing times: 50 s, 100 s, 150 s, 200 s, 250 s, and 300 s.

Another interesting observation was the impact of annealing temperature on the zinc concentration in the grain. When the annealing temperature increased, its impact on the zinc concentration did not show a clear trend. At the beginning of the process, with annealing times of 50 and 100 s, as the annealing temperature increased from 350 K by 2 degrees, the change in zinc concentration was similar to that observed when the temperature increased by 0.5 K from 353.5 K, and twice as large as when it increased by 0.5 K from 353 K. In the middle of the process, with an annealing time of 150 s, the differences in zinc concentration between annealing temperatures of 350 K and 352 K were

very small, whereas the differences between annealing temperatures of 352 K and 353 K were huge. At the end of the analysis, the differences in Zn concentration between annealing temperatures of 350 K and 352 K were similar to those between annealing temperatures of 353 K and 354 K. However, the differences in Zn concentration in the grain between annealing temperatures of 352 K and 353 K were again the largest, being almost 2.5 times larger than those mentioned earlier.

5. Summary and Conclusions

The mathematical model and the numerical simulation prepared for the amorphous $\text{Mg}_{72}\text{Zn}_{28}$ alloy allowed for efficient calculations of the grain growth in the primary phase, α -Mg, and the zinc concentration in the grain and amorphous phase.

At an isothermal annealing temperature of 354 K, the grain size changed from 20 to 70 nm after 300 s. A very good agreement between the simulation results (70 nm) and the experimental results (about 71 nm) was observed.

The grain growth kinetics were greater with higher values of the isothermal annealing temperature. It should be noted that the diffusion process is very slow, and the nucleation process may still progress, which may lead to a situation in which the grain size will be very small, e.g., about 50 nm.

At different annealing temperatures, the grain growth rates were different, as observed in the simulation results. Similarly, different zinc concentrations were calculated in grains at different annealing temperatures, and their change rates changed during the process.

Author Contributions: Conceptualisation, J.L.; methodology, J.L., P.L.Ż. and V.V.; software, P.L.Ż.; investigation, B.O. and V.V.; formal analysis, J.L., P.L.Ż., B.O. and V.V.; data curation, B.O., P.L.Ż., J.L. and V.V.; writing—original draft, B.O. and J.L.; writing—review and editing, P.L.Ż. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by “The Excellent Initiative—Research University” (IDUB) programme, grant number 501.696.7996 (action 4, 1658) and AGH project no 16.16.170.7998/B307.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The raw data supporting the conclusions of this article will be made available by the authors on request.

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. Murr, L.E. Computer Simulations in Materials Science and Engineering. In *Handbook of Materials Structures, Properties, Processing and Performance*; Springer International Publishing: Cham, Switzerland, 2016; pp. 1–15.
2. Ericsson, A.; Fisk, M. Modeling of Diffusion-Controlled Crystallization Kinetics in Al-Cu-Zr Metallic Glass. *Metals* **2022**, *12*, 867. [\[CrossRef\]](#)
3. Stefanescu, D. Critical Review of the Second Generation of Solidification Models for Castings: Macro Transport—Transformation Kinetics Codes. In *Proceedings of the Conference: Modeling of Casting and Welding Processes VI*, Palm Coast, FL, USA, 21–26 March 1993.
4. Szopa, R. *Modelowanie Krzepnięcia i Krystalizacji z Wykorzystaniem Kombinowanej Metody Elementów Brzegowych*; Wydawnictwo Politechniki Śląskiej: Gliwice, Poland, 1999.
5. Uhlmann, D. A kinetic treatment of glass formation. *J. Non-Cryst. Solids* **1972**, *7*, 337–348. [\[CrossRef\]](#)
6. Morris, D. Glass formation and crystallisation in NiSiB alloys—I. Glass formation-test of the “avoidance of crystallisation” approach. *Acta Metall.* **1983**, *31*, 1479–1489. [\[CrossRef\]](#)
7. Thompson, C.V.; Spaepen, F. On the approximation of the free energy change on crystallization. *Acta Metall.* **1979**, *27*, 1855–1859. [\[CrossRef\]](#)
8. Gránásky, L. Quantitative analysis of the classical nucleation theory on glass-forming alloys. *J. Non-Cryst. Solids* **1993**, *156–158*, 514–518. [\[CrossRef\]](#)
9. Ge, L.; Hui, X.; Wang, E.; Chen, G.; Arroyave, R.; Liu, Z. Prediction of the glass forming ability in Cu–Zr binary and Cu–Zr–Ti ternary alloys. *Intermetallics* **2008**, *16*, 27–33. [\[CrossRef\]](#)

10. Yang, W.; Liu, F.; Liu, H.; Wang, H.; Chen, Z.; Yang, G. Glass forming ability in Cu–Zr binary alloy: Effect of nucleation mode. *J. Alloys Compd.* **2009**, *484*, 702–707. [[CrossRef](#)]
11. Tanner, L.; Ray, R. Metallic glass formation and properties in Zr and Ti alloyed with Be—I the binary Zr–Be and Ti–Be systems. *Acta Metall.* **1979**, *27*, 1727–1747. [[CrossRef](#)]
12. Masuhr, A.; Waniuk, T.A.; Busch, R.; Johnson, W.L. Time Scales for Viscous Flow, Atomic Transport, and Crystallization in the Liquid and Supercooled Liquid States of $\text{Zr}_{41.2}\text{Ti}_{13.8}\text{Cu}_{12.5}\text{Ni}_{10.0}\text{Be}_{22.5}$. *Phys. Rev. Lett.* **1999**, *82*, 2290–2293. [[CrossRef](#)]
13. Ericsson, A.; Pacheco, V.; Sahlberg, M.; Lindwall, J.; Hallberg, H.; Fisk, M. Transient nucleation in selective laser melting of Zr-based bulk metallic glass. *Mater. Des.* **2020**, *195*, 108958. [[CrossRef](#)]
14. Suryanarayana, C.; Inoue, A. *Bulk Metallic Glasses*; CRC Press: Boca Raton, FL, USA, 2017.
15. Köster, U.; Herold, U. *Crystallization of Metallic Glasses*; Springer: Berlin/Heidelberg, Germany, 1981; pp. 225–259.
16. Chen, Q.; Jeppsson, J.; Ågren, J. Analytical treatment of diffusion during precipitate growth in multicomponent systems. *Acta Mater.* **2008**, *56*, 1890–1896. [[CrossRef](#)]
17. Kampmann, R.; Eckerlebe, H.; Wagner, R. Precipitation Kinetics in Metastable Solid Solutions—Theoretical Considerations and Application to Cu–Ti Alloys. *MRS Online Proc. Library* **1985**, *57*, 525–542. [[CrossRef](#)]
18. Myhr, O.; Grong, O. Modelling of non-isothermal transformations in alloys containing a particle distribution. *Acta Mater.* **2000**, *48*, 1605–1615. [[CrossRef](#)]
19. Porter, D.A.; Easterling, K.E. *Phase Transformations in Metals and Alloys*; Taylor & Francis Group, CRC Press: Boca Raton, FL, USA, 1981.
20. Cahn, R.; Haasen, P. *Physical Metallurgy*; Elsevier Science: Amsterdam, The Netherlands, 1996.
21. Wagner, R.; Kampmann, R.; Voorhees, P.; Kosterz, G. *Homogeneous Second Phase Precipitation: Phase Transformations in Materials Science and Technology*; Wiley-VCH: Weinheim, Germany, 2001.
22. Wagner, R.; Kampmann, R.; Voorhees, P.W., Homogeneous Second-Phase Precipitation. In *Materials Science and Technology*; John Wiley & Sons, Ltd.: Hoboken, NJ, USA, 2013.
23. Langer, J.S.; Schwartz, A.J. Kinetics of nucleation in near-critical fluids. *Phys. Rev. A* **1980**, *21*, 948–958. [[CrossRef](#)]
24. Patankar, S.V. *Numerical Heat Transfer and Fluid Flow*; Hemisphere Publishing Corporation: London, UK, 1980.
25. Kapturkiewicz, W.; Frasz, E.; Burbelko, A. Why is the computer modelling needed in casting? *Przegląd Odlewnictwa* **2005**, *55*, 15–23.
26. Fourier, J. *Theorie Analytique de la Chaleur*; Didot: Paris, France, 1822.
27. Fick, D.A. V. On liquid diffusion. *Lond. Edinb. Dublin Philos. Mag. J. Sci.* **1855**, *10*, 30–39. [[CrossRef](#)]
28. Tanzilli, R.; Heckel, R. Numerical solutions to the finite, diffusion-controlled, two-phase, moving-interface problem (with planar, cylindrical, and spherical interfaces). *AIME Trans.* **1968**, *242*, 2312–2321.
29. Kammerer, C. *Interdiffusion and Impurity Diffusion in Magnesium Solid Solutions*; University of Central Florida: Orlando, FL, USA, 2013.
30. Opitek, B.; Gracz, B.; Lelito, J.; Krajewski, W.K.; Łucarz, M.; Bała, P.; Kozieł, T.; Gondek, L.; Szucki, M. Crystallization Kinetics Analysis of the Binary Amorphous $\text{Mg}_{72}\text{Zn}_{28}$ Alloy. *Materials* **2023**, *16*, 2727. [[CrossRef](#)] [[PubMed](#)]

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.