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THERMALLY INDUCED STRUCTURAL TRANSFORMATIONS OF MULTICOMPONENT $Fe_{72}Cu_1V_4Si_{15}B_8$ ALLOY

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ABSTRACT
Thermally induced structural transformations of $Fe_{72}Cu_1V_4Si_{15}B_8$ alloy were examined. Thermal analysis revealed multistep structural stabilization process starting at around 470 °C, manifested by two complex exothermic DTA peaks, which were deconvoluted. Microstructure of the as-prepared and thermally treated alloy was studied using XRD. Kinetic triplets of individual steps were determined and further checked by comparing simulated and experimental DTA curves.

INTRODUCTION
Nanocrystalline alloys, obtained from the amorphous precursors, have been widely studied in recent time due to many applications based on their favorable functional properties [1,2]. Thermodynamic and kinetic metastability of these materials allow the controlled heat treatment to be used to obtain materials with targeted microstructure and morphology, convenient for many technologically interesting applications. In that way it is possible to obtain nanocrystalline alloys with better functional properties than the purely amorphous and purely crystalline ones. This can be achieved starting with amorphous precursors by controlling the rates of nucleation and crystal growth and by proper choice of chemical composition of the alloy and thermal treatment procedure.

EXPERIMENTAL
The nanocrystalline samples of the $Fe_{72}Cu_1V_4Si_{15}B_8$ alloy were prepared by melt-spinning method. The obtained alloy samples were ribbon-shaped, 2 mm wide and 40 μm thick.

DTA measurements at constant heating rates (5,10, 20 °Cmin^{-1}) were conducted to study thermally induced structural transformations of the alloy. TA SDT 2960 instrument was used to this purpose. Measurements were done under helium atmosphere to prevent the oxidation of material. Complex DTA peaks were deconvoluted into several peaks using Origin Pro 8.5 software applying Gaussian Lorentzian cross-product function.

XRD data were collected at room temperature using Philips PW-1710 automated diffractometer with Cu K_α line, operated at 40 kV and 30 mA. Thermal treatment of the samples subjected to XRD analysis included isothermal annealing under argon atmosphere, at different temperatures.

RESULTS AND DISCUSSION

The influence of thermal treatment on the structure of the multicomponent nanostructured $Fe_{72}Cu_1V_4Si_{15}B_8$ alloy was investigated in the temperature range 25-800 °C. It was shown that the alloy was stable up to around 470 °C when structural transformations started, manifested as two well separated exo maxima, reflecting the processes of crystallization and growth of the formed crystallites, Fig. 1a.

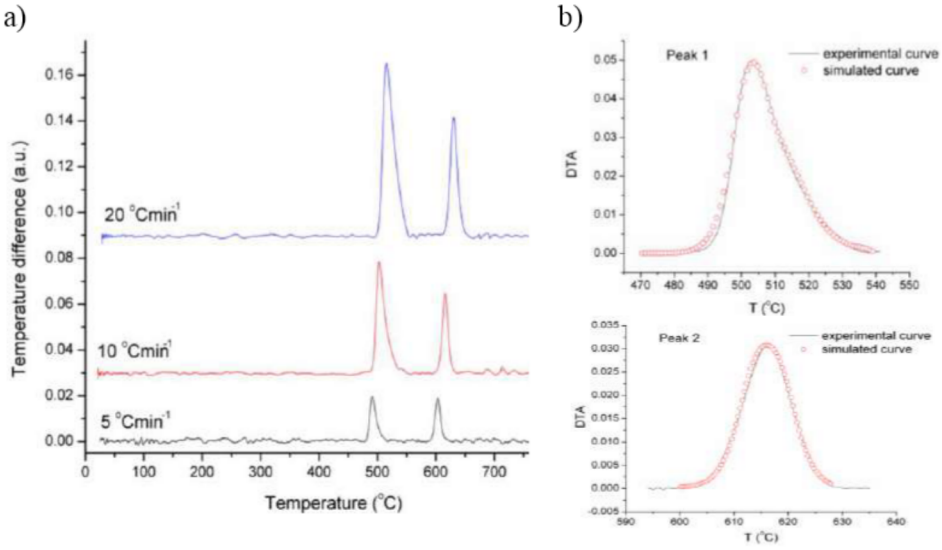

Figure 1. a) Baseline-corrected DTA curves for different heating rates; b) DTA curves, experimental and simulated, based on kinetic triplets for 10 °Cmin^{-1}.

The X-ray diffractogram of initial alloy, Fig.2a, revealed the presence of both the amorphous and crystalline phases. It was shown that the α-Fe(Si) phase is the dominant one (crystallite size 40nm) while the metastable Fe_3B

crystalline phase is the minor one. On the other hand, the alloy isothermally treated at 700 °C for 210 min was completely crystalline, containing two solid solutions with different percentages of Si and one with relatively high V content, and Fe_2B phase, Fig. 2b. This result is in good accordance with EDAX (results aren't presented here).

With a view to determining kinetic triplets of individual crystallization steps, complex DTA peaks were deconvoluted. In this way we obtained four well formed peaks corresponding to single step processes of crystallization of different phases. Kinetic parameters, obtained by using Kissinger's and Ozawa's methods, Table 1, correspond to simultaneous correlated movements of large number of atoms during transformations. The presence of considerable number of quenched-in nuclei in the initial alloy provokes considerably lower value of apparent activation energy of crystallization of α-Fe phase, in comparison with the similar systems [3].

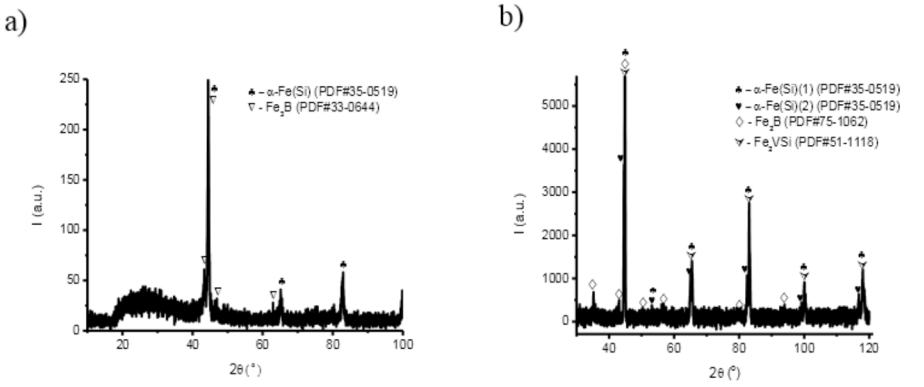

Figure 2. a) XRD of the as-prepared $Fe_{72}Cu_1V_4Si_{15}B_8$ alloy; b) XRD of the alloy sample thermally treated at 700 °C for 210 min.

Conversion function, f(α), was found by application of Málek's method [4]. This method suggested that empirical Šesták-Berggren model [5] can be used for description of the individual steps, as presented in Table 1. The determined kinetic triplets were applied to simulate experimental DTA curves. Comparison of simulated DTA curves, calculated using the determined kinetic triplets, and experimental DTA curves Fig. 1b showed very good accordance with correlation factor of 0,99. In this way obtained kinetic triplets can be used to predict the lifetime and the rate of processes for initial material as well as for partially or fully crystallized materials, which is very important for their application in electronics.

Table 1. Kinetic triplets of individual crystallization steps

	Experimental peak 1		Experimental peak 2	
Method	Step 1	Step 2	Step 1	Step 2
Kissinger, E_a (kJ/mol)	281 ± 1	248 ± 4	346 ± 4	322 ± 1
Ln(A/min^{-1})	43.0 ± 0.1	37.3 ± 0.8	46.3 ± 0.8	42.7 ± 0.1
Ozawa, E_a (kJ/mol)	280 ± 1	248 ± 4	343 ± 4	320 ± 1
Ln(A/min^{-1})	42.8 ± 0.1	37.3 ± 0.5	46.0 ± 0.6	42.4 ± 0.1
f(α)	$\alpha^{0.48}(1-\alpha)^{0.83}$	$\alpha^{0.89}(1-\alpha)^{1.34}$	$\alpha^{0.79}(1-\alpha)^{1.0}$	$\alpha^{0.79}(1-\alpha)^{1.0}$

CONCLUSION

Thermal treatment of nanocrystalline $Fe_{72}Cu_1V_4Si_{15}B_8$ alloy induces multi-step thermal stabilization process at temperatures higher than 470 ºC. This process includes, beside the nucleation, the growth of the present nuclei and recrystallization, yielding α-Fe solid solutions with different contents of Si and V and Fe_2B phase as the final products. Lower values of apparent activation energy of crystallization in comparison with the similar systems originate from the presence of significant number of quenched-in nuclei in the as-prepared alloy. The determined values of kinetic parameters and conversion functions of individual steps fit very well experimental DTA curves, and can be used to predict lifetime of the material in different stages of crystallization and the rate of the process in different temperature regions.

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REFERENCES

[1] C. Suryanarayana, A. Inoue, International Materials Reviews, 2013, **58**, 131-166.
[2] T. Kulik, Journal of Non-Crystalline Solids, 2001, **287**, 145-161.
[3] M. Vasić, D.M. Minić, V.A. Blagojević, D.M. Minić, Thermochimica Acta, 2013, **562**, 35-41.
[4] J. Málek, Thermochimica Acta, 2000, **355**, 239-253.
[5] J. Šesták, G. Berggren, Thermochimica Acta, 1971, **3**, 1-12.

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