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Kinetic model of the crystallization process of $Cu_{46}Zr_{50}Al_4$ metallic glass

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Abstract

Nanocomposite materials based on the Cu-Zr glass-forming system, which are an amorphous matrix with crystalline inclusions of the cubic B2 phase of the CuZr compound, are promising structural materials due to their unique mechanical properties. One of the methods for producing such materials is the heat treatment of amorphous samples. To develop optimal conditions for such processing, it is necessary to study the kinetics of crystallization of amorphous copper-zirconium. In this work, the crystallization processes, structure and thermal properties of the amorphous $Cu_{46}Zr_{50}Al_4$ alloy, obtained by suction casting were studied for the first time in a wide temperature range from room temperature up to 600 °C. We reveal the complex character of the crystallization process of this alloy described by a three-step sequential reaction. Using a comprehensive approach, including calorimetric studies, X-ray phase analysis and kinetic modeling by multivariate nonlinear regression, we develop the kinetic model and estimate kinetic parameters of the crystallization processes in the alloy. We find that the best description of the experimental data is achieved when autocatalytic equations are used to model crystallization processes: a heterogeneous n-th order reaction with autocatalysis, as well as the Prout-Tompkins equation. The found activation energy of crystallization of the alloy is E_a = 387.59 kJ/mol. Based on the results obtained, we propose a procedure for fabricating the nanocomposite materials by heating an amorphous alloy up to temperatures of about 420-460 °C.

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