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Applicability of Kissinger's Relation in the Determination of Activation Energy of Amorphous $Fe_{76}Dy_4B_{20}$ Alloy

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Abstract—*Applicability of Kissinger's relation in the determination of activation energy of amorphous $Fe_{76}Dy_4B_{20}$ alloy was studied by Differential Scanning Calorimetry (DSC) . The activation energy (E_a) of crystallization, and Frequency factor (k_o)were calculated using three models namely Kissinger, Augis-Bennet and Matusita-Sakka. The average activation energy for primary crystallization of amorphous $Fe_{76}Dy_4B_{20}$ alloy using the above three methods is found to be 578.59 kJouls/mole. The frequency factor of amorphous $Fe_{76}Dy_4B_{20}$ alloy using Kissinger method is found to be $8.5x10^{31}$ $(sec)^{-1}$.*

Keywords: *differential scanning calorimetry, activation energy, crystallization temperature*

1. INTRODUCTION

The theory of crystallization in amorphous materials can be explained by considering the structure and the kinetics of the crystallization. Therefore, the investigation of crystallization kinetics is important since it quantifies the effect of the nucleation and growth rate of the resulting crystallites [1]. Crystallization kinetics of amorphous materials was investigated by explaining the crystallization mechanism and the crystallization activation energy in terms of isothermal and non isothermal methods with different approaches. Different thermal analysis techniques used in crystallization kinetic studies were presented and a correlation between kinetic and structural investigations was made to determine the crystallization mechanism [2,3]. In this paper, we present the applicability of Kissinger's relation[4] in the determination of activation energy of amorphous $Fe_{76}Dy_4B_{20}$ alloy.

2. EXPERIMENTAL

Commercially available specimens of amorphous $Fe_{76}Dy_4B_{20}$ ribbons prepared by single roller melt spinning technique under inert atmosphere were procured. The alloy ribbons were about 1 mm wide and about 30 µm thick. Amorphous nature of the ribbons was confirmed by X-ray diffraction (XRD). The as-quenched sample of $Fe_{76}Dy_4B_{20}$ ribbon was heated in DSC (DSC-50, Shimadzu, Japan) at four linear heating rates (10, 20, 30 and 40 Kelvin/min) from room temperature to 950 K. The DSC scans were recorded by a thermal analyzer interfaced to a computer.

3. RESULTS AND DISCUSSION

According to Kissinger's method [4,5], the transformation under non-isothermal condition is represented by a first-order reaction. More over, the concept of nucleation and growth has not been included in Kissinger equation. Matusita et al.[6] have developed a method on the basis of the fact that crystallization does not advance by an n^{th} order reaction but by a nucleation and growth process. They emphasized that crystallization mechanism such as bulk crystallization or surface crystallization should be taken into account for obtaining activation energy. Augis and Bennett method [7] is helpful in obtaining kinetic parameters such as frequency factor (k_0) along with activation energy (E_a) of crystallization and therefore preferred for the calculation of the kinetics over the other models.

The DSC curves of as-quenched $Fe_{76}Dy_4B_{20}$ sample at four heating rates of crystallization are shown in Fig. 1.

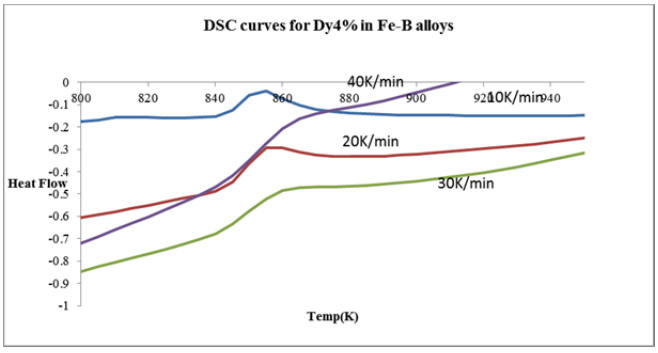

Fig. 1: The DSC curve of amorphous $Fe_{76}Dy_4B_{20}$ ribbon four heating rates of crystallization in the temperature range 800 K – 940 K

Determination of activation energy using Kissinger method

The activation energy for crystallization of an amorphous alloy under a linear heating rate can be estimated using Kissinger's peak shift method, which relates the peak temperature, T_p, with heating rate (β) through the equation

$$\ln (\beta/T_p^2) = -(E_a/RT_p) + \ln(k_0R/E_a) \text{----------(1)}$$

where E_a is the activation energy for crystallization, T_p the peak temperature and k_0 the frequency factor which is defined as the number of attempts made by the nuclei per second to overcome the energy barrier. This also provides information for the calculation of number of nucleation sites, present in the material for crystal growth [8].

Fig. 2 shows the graph of ln (β/T_p^2) vs. 1000/ T_p which is a straight line with a slope ($-E_a/R$) and an intercept of ln (k_0R/E_a). The activation energy and the frequency factor k_0 for crystallization peak are given in Table 1.

Table1

COMPOSITION	Activation Energy E_a kJouls/mole				Frequency factor $(sec)^{-1}$	
	Kessinger's Method	Augis-Bennet's Method	Matusita-Sakka's Method	Average E_a KJouls/mole	Kessinger's Method	Augis-Bennet's Method
$Fe_{76}Dy_4B_{20}$	571.3	578.488	586.08	578.59	$8.5x10^{31}$	$2.92x10^{33}$

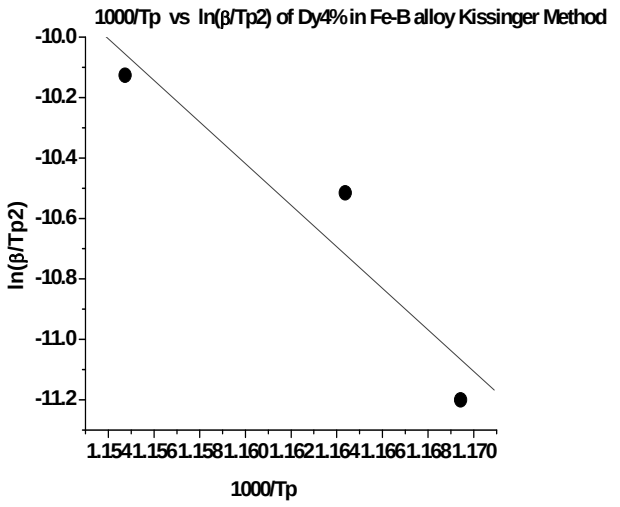

Fig. 2: ln (β/T_p^2) vs. (1000/ T_p) of amorphous $Fe_{76}Dy_4B_{20}$ alloy

Determination of activation energy using Augis & Bennett Method

The activation energy for crystallization of an amorphous alloy under a linear heating rate can be estimated using Augis & Bennett method, which relates the peak temperature, T_p, with heating rate (β) through the equation

$$\ln(\beta/T_p) = -E_a/RT_p + \ln k_o \text{----------(2)}$$

where E_a is the activation energy for crystallization, T_p the peak temperature and k_0 the frequency factor. Fig. 3 shows the graph of ln (β/T_p) vs. $1000/T_p$ which is a straight line with a slope ($-E_a/R$) and an intercept of ln k_0. The activation energy E_a and the frequency factor k_0 for crystallization peak are also given in Table 1.

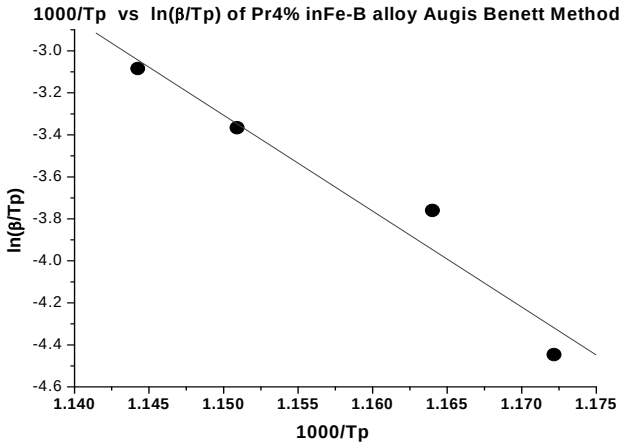

Fig. 3 ln (β/T_p) vs. (1000/ T_p) of amorphous $Fe_{76}Pr_4B_{20}$ alloy

Determination of activation energy using Matusita-Sakka Method

The activation energy for crystallization of an amorphous alloy under a linear heating rate can also be estimated using **Matusita-Sakka**'s peak shift method, which relates the peak temperature, T_p, with heating rate (β) through the equation

$$\ln (\beta) = -(E_a/RT_p) + \text{constant----------(3)}$$

where E_a is the activation energy for crystallization, T_p the peak temperature and R is the universal gas constant. Fig. 4 shows the graph of ln (β) vs $1000/T_p$ which is a straight line with a slope ($-E_a/R$) . The activation energy is given in Table 1.

The slight difference in the activation energy calculated using different models may be attributed to the different approximations used in the models. Thus, the average activation energy (E_a) and the frequency factor of amorphous $Fe_{76}Dy_4B_{20}$ alloy are 578.59 kJouls/mole and $8.5x10^{31}$ $(sec)^{-1}$, respectively.

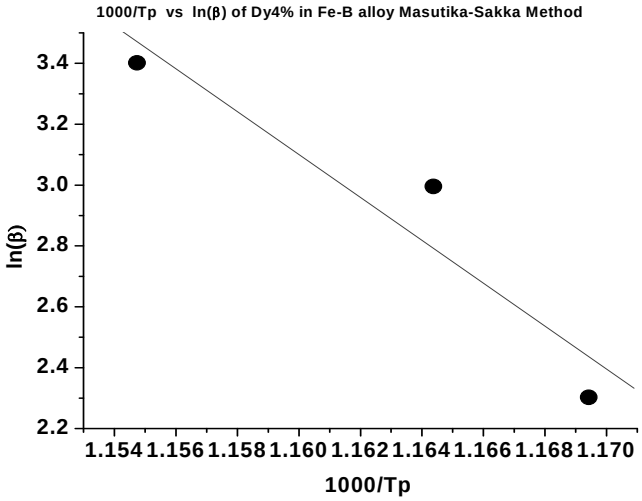

Fig. 4 ln (β) vs. (1000/ T_p) of amorphous $Fe_{76}Dy_4B_{20}$ alloy

4. CONCLUSIONS

The average activation energy for primary crystallization of amorphous $Fe_{76}Dy_4B_{20}$ alloy using Kissinger, Augis-Bennet and Matusita-Sakka methods is found to be 578.59 kJouls/mole. The frequency factor of amorphous $Fe_{76}Dy_4B_{20}$ alloy using Kissinger method is found to be $8.5x10^{31}$ $(sec)^{-1}$. The above values are in good agreement with values of other similar systems.

5. ACKNOWLEDGEMENTS

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