Model approaches to overall crystallization

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Thermal analysis (DTA, DSC, TGA) is the basic method detecting the temperature, heat flow or mass change when the phase transition occurs. During the crystallization, the heat of fusion is released and that is why the temperature change at crystallization is detected. An amount of released heat needs to be sufficiently high to influence temperature and thus this method detects the overall crystallization. Model approaches of the thermal analysis data are usually based on the Johnson-Mehl-Avrami-Kolmogorov (JMAK) model, when crystallization fraction $X(t) = V_c(t)/V_0 = 1 - exp[-V_{ex}(t)/V_0]$, where V_0 is the initial volume of the melt, $V_c(t)$ is the volume of the crystalline phase at time t and V_{ex} denotes so-called extended volume. JMAK model presumes that crystallization occurs by nucleation (homogeneous or heterogeneous) and successive growth. In consequence of crystallization, volume of the melt decreases with time as V_c increases, and to take into account this depletion is rather difficult and thus V_{ex}, which represents the volume of the crystalline phase if overlap among the growing nuclei is disregarded, was introduced. JMAK model is widely used in thermal analysis though model assumptions are not often fulfilled.

In this work aluminum (Al) crystallization was detected by simultaneous thermal analyzer Setaram Setsys Evolution 16 at isothermal conditions (multiple isotherms were studied). Obtained experimental data were analyzed by two methods: (I) JMAK model and (ii) numerical solution of the kinetic equations of homogeneous nucleation to determine the crystallization fractions of Al crystallization including melt depletion at crystallization. Comparison of these models enabled us to verify if the JMAK model approach was justified.