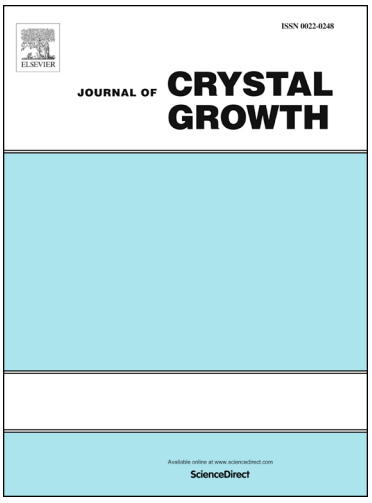


# Monte Carlo simulation of induction time and metastable zone width; stochastic or deterministic?

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# Monte Carlo simulation of induction time and metastable zone width; stochastic or deterministic?

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**Abstract**

The induction time and metastable zone width (MSZW) measured for small samples (say 1 mL or less) both scatter widely. Thus, these two are observed as stochastic quantities. Whereas, for large samples (say 1000 mL or more), the induction time and MSZW are observed as deterministic quantities. The reason for such experimental differences is investigated with Monte Carlo simulation. In the simulation, the time (under isothermal condition) and supercooling (under polythermal condition) at which a first single crystal is detected are defined as the induction time $t$ and the MSZW $\Delta T$ for small samples, respectively. The number of crystals just at the moment of $t$ and $\Delta T$ is unity. A first crystal emerges at random due to the intrinsic nature of nucleation, accordingly $t$ and $\Delta T$ become stochastic. For large samples, the time and supercooling at which the number density of crystals $N/V$ reaches a detector sensitivity $(N/V)_{\mathrm{det}}$ are defined as $t$ and $\Delta T$ for isothermal and polythermal conditions, respectively. The points of $t$ and $\Delta T$ are those of which a large number of crystals have accumulated. Consequently, $t$ and $\Delta T$ become deterministic according to the law of large numbers. Whether $t$ and $\Delta T$ may stochastic or deterministic in actual experiments should not be attributed to change in nucleation mechanisms in molecular level. It could be just a problem caused by differences in the experimental definition of $t$ and $\Delta T$.

**Keywords**

A1. Nucleation,

A1. Monte Carlo simulation

A1. Induction time

A1. Metastable zone width

A2. Industrial crystallization

## 1. Introduction

The induction time is generally defined as the time elapsed from the moment of achievement of supersaturation to the moment of detection of "first crystallization event" [1]. In the measurement of induction time, the temperature or supercooling is kept constant (isothermal). The metastable zone width (MSZW) is similarly defined as the supercooling when a "first crystallization event" is detected under the polythermal (increasing supercooling) condition. Although there is a difference in temperature profile, both induction time and MSZW are nucleation-related physical quantities and are considered as barometer of the difficulty of nucleation.