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STRUCTURE FUNCTION CALCULATIONS FOR OSTWALD RIPENING PROCESSES

Prepared By:	Razi A. Hassan
Academic Rank:	Assistant Professor
University and Department:	Alabama A&M University Chemistry
NASA/MSFC:	
Laboratory:	Space Science
Division:	Microgravity Science & Applications
Branch:	Chemistry and Polymeric Materials
MSFC Colleague:	Dr. J. Patton Downey Dr. Donald Frazier
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ABSTRACT

A program for computing the Structure Function for configurations involved in Ostwald Ripening has been written. The basic algorithms are derived from a mathematical analysis of a two-dimensional model system developed by Bortz, et. al (1974).

INTRODUCTION

The Chemistry and Polymeric Sciences Branch conducts experimental and theoretical research to advance the science and technology of organic and polymeric materials having applications as optical and other important devices. Studies relate to gravitational influences on solidification, crystal-growth, thin film growth, and polymerization of such materials. Space laboratories in free-fall around the earth offer an environment in which body forces on fluids can be minimized over a relatively extended period of time and range of experimental conditions. Other advantages include a quiesent environment allowing for the growth of defect-free crystals. A fundamental understanding of these low-gravity growth processes can lead to better understanding of metal fatigue in alloys, the behavior of fogs and aerosols, and, in general, almost any of the multiphase systems which covers a broad range of technology.

When a homogenous melt containing two components is cooled to a temperature at which the two components are no longer totally miscible, the melt separates into phases of differing compositions. Although equilibrium compositions are predictable by the system's phase diagram, there is no way to predict phase distribution during alloy formation. Distribution of phases is an important aspect of materials properties. Important mechanisms determining distribution on earth are sedimentation and convection. Under low-gravity conditions, sedimentation and convection dominate, affecting morphology. One such separation process is **Ostwald Ripening.**

Ostwald Ripening is a process by which larger droplets grow at the expense of smaller ones by the diffusion of mass away from droplets below a critical radius toward ones above this size. This phenomenon is important in many disciplines involving multiphase components, including long-term metal alloy integrity, foam stability, and weather phenomena. The Branch is leading a research program to perform a flight experiment which will provide data on the ripening process where gravity effects have been eliminated.

In order to draw a picture of Ostwald Ripening, imagine a solution containing two chemical components. The solution is supersaturated

with solute, and nuclei of a second phase have already started to grow. The supersaturated solution shall be called the parent phase, and the nuclei shall be termed the second phase. The nuclei shall be assumed to be large enough to have well-defined surfaces so that macroscopic theories such as thermodynamics can be applied. Such nuclei shall be called grains. Of interest to us is the grain size dustribution, which we will represent by a Structure Function.

The Structure Function can be defined as follows: The superposition of waves of different amplitudes and phases can be accomplished by vectorial addition. If f_1 and f_2 are the amplitudes of waves scattered by atoms 1 and 2, and ϕ_1 and ϕ_2, are the phases, the resultant amplitude is:

$$F = f_1\phi_1 + f_2\phi_2$$

In 3 dimensions:

$$F(hjk) = \sum_j f_j e^{2\pi i(hxj/a + jYj/b + kzj/c)}$$

where h,j,k are the Miller indices of the crystal.

The expression F(hjk) is called the structure function of the system. Its value is determined by the exponential terms, which also reflect the cluster sizes of the grains formed during Ostwald Ripening.

PROCEDURE

For our computer simulation, we start with an initial state at t=0 from a completely random configuration of A and B particles. We then follow the time evolution of the random varible x_t representing the state of the system at time t. The stochastic process, an example of a Monte Carlo simulation, describing the evolution of x_t is Markovian. The algorithm used to generate our program was developed from a paper by Bortz (1974). The structure function, S(k,t), is defined as follows:

$$S(\vec{k},t) = \sum_{\vec{r}} e^{i\vec{k} \times \vec{r}}\, G(\vec{r},t)$$

$$\vec{k} = \frac{2}{80}\vec{\mu}$$

$$\vec{\mu} = (\mu x, \mu y)$$

$$G(\vec{r},t) = n^{-1}\sum_i [\eta(\vec{r}_i)\eta(\vec{r}_i - \vec{r}) - \bar{\eta}^2]$$

$$\vec{\eta} = n^{-1}\Sigma\eta_i$$

$N = N_A + N_B$

N_A = the number of A type particles

N_B = the number of B type particles

$\vec{r}$ = describes the different positions of the system at times t.

CONCLUSION

While we expect that the values from our computer simulations will reflect Ostwald Ripening, at this point the program is still being tested. Some preliminary runs seem to justify our expectations.

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