# NANO-SCALE SOLIDIFICATION PHENOMENA

J. Czerwinska*, E. Deriaz* & T. A. Kowalewski*
*Institute of Fundamental Technological Research, Polish Academy of Science, Warsaw, Poland

*Summary* Understanding of macro-scale solidification processes can benefit in a significant way from the information in the nano-scale. This papers presents a way to investigate nano-scale solidification by Molecular Dynamics simulations. Macro-scale parameters can be extracted from the nano-scale simulations to obtain understanding about the fully multi-scale characteristics of solidification phenomena.

## INTRODUCTION

Solidification is a complex multi-physics transition phenomena which is highly important for various industrial applications. It is a multi-scale process and some aspects of it can be much easier investigated by theory and numerical simulations than experiments. Experimental studies of solidification in nano-scale are both costly and difficult to perform. Molecular Dynamics simulation offers a simple and comprehensive tool to understand the complex microscopic phenomena occurring in solidification process. We have been investigating solidification of one and multi component Lennard-Jones crystals growth. The numerical virtual solidification facility performs calculations in two steps. First simulations study time dependent solidification process which results in the solid material sample. Next the sample is undergoing further simulation tests to obtain its material characteristics and properties such as strain-stress relation. These procedure allows to study following properties: local order parameter to decide if the sample is fluid or solid, the formation of the nucleation sites, the orientation and order of the crystal structure, the velocity of the solidification front, the presence and characteristics of voids in the crystal structure, the deformation parameter, the elasticity and the shear-stress response of a material, the transport coefficients of the media including the self-diffusion coefficients and the viscosity of liquid during the solidification. The presented investigation is a first step to develop virtual facility for multi-scale solidification studies. Nano-scale parameters will be later on implemented into the continuum models to provide comprehensive view of the multi-scale effects in solidification.

## SOLIDIFICATION IN NANO-SCALE

Molecular Dynamics simulations allow to observe formation of the solidification during the time period. This allows to study formation of nucleation sides and movement of solidification front. Such studies has been performed for one and multicomponent materials. Figure 1 shows cut through material of four component Lennard-Jones crystal. Figure 2 presents differences in the crystal formation. In both figure it can be notices that in specific condition crystal structure has void regions due to the conditions on which the solidification was performed, mainly the difference in the temperature gradient during the cooling process. Such imperfection in crystal structure are very difficult to study experimentally. However, numerical simulation give insight to such processes. There is a possibility to obtain temperature gradient relation with the structure of the crystal network. This also allows to verify solid parameters and sample strength. It has to be noted that the multicomponent materials have had similar behaviour as one component material in terms of the influence of the temperature gradient on the void formation. Moreover crystal formation depends very strongly on the boundary conditions, mainly if the solidifying fluid is completely or partially confined in the solid structure.

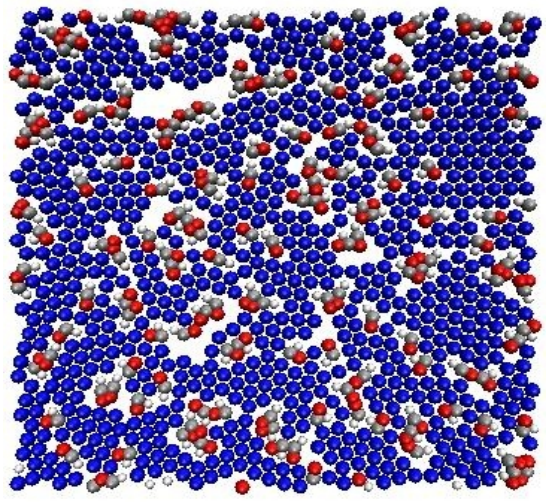
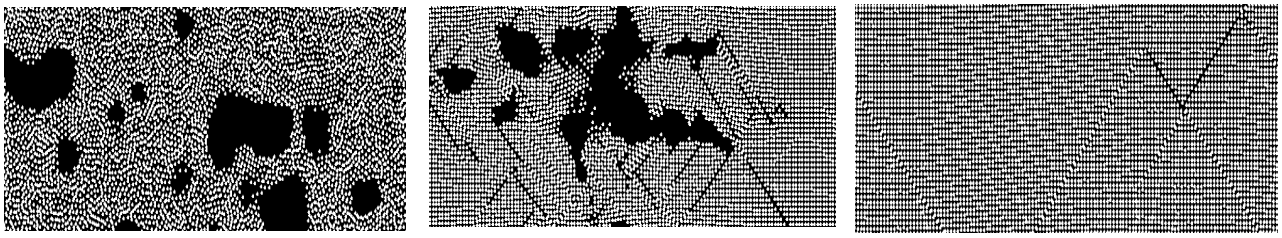


Figure 1: Four component Lennard-Jones crystal.



a) b) c)

Figure 2: Characteristics of material depending on the solidification procedure: a) solid boundary at one end; b) high temperature gradient (rapid crystallization); c) homogeneous and small temperature gradient (slow crystallization).

## MACROSCALE PARAMETERS

Macro-scale parameters were obtained from nano-scale solidification simulations by several numerical experiments. The properties measured during the nano-scale solidification are mentioned in introduction. Here, only few example are briefly presented. The solidified material strength was measured by implementing force (see Figure 3) . This has lead to the strain-stress relation presented for one component Lennard-Jones crystal on Figure 4.

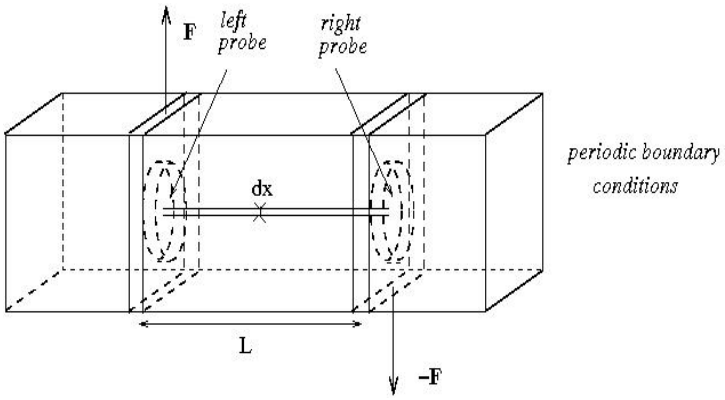



Figure 3: Illustration for the material strength test.

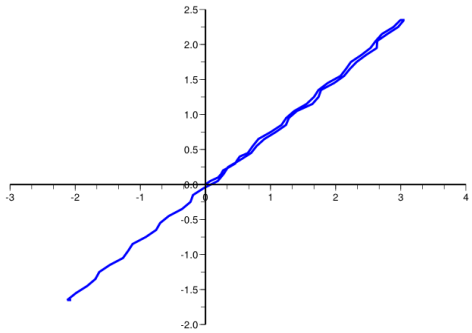


Figure 4: Strain-stress relation for homogeneous Lennard-Jones crystal.

Next two figures present example of calculation of liquid macroscopic parameters such as diffusion coefficient and its development during the solidification process.

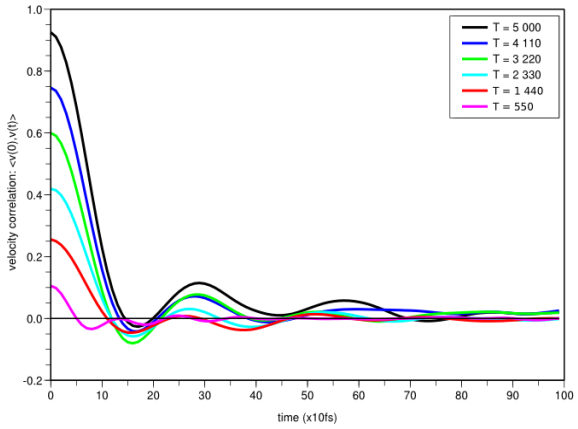



Figure 5: Green-Kubo estimation of diffusion in liquid under solidification. The values are given in Lennard-Jones units. The figure presents correlation function for various temperature gradient, which refers to different molecules mobility. Similarly viscosity and thermal conductivity can be obtained.

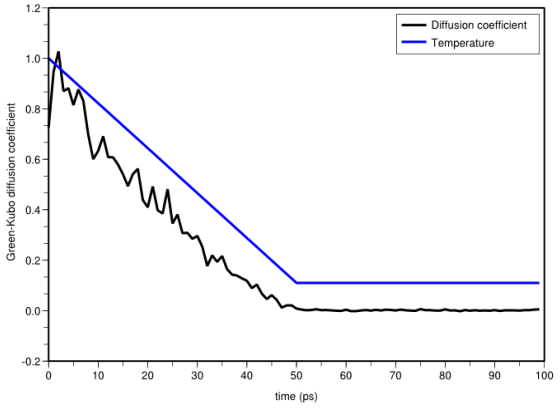



Figure 6: Average diffusion coefficient and the time history during the solidification process. The figure also shows temperature changes in the sample.

## CONCLUSIONS

In this paper briefly were presented methods to perform and verify nano-scale solidification. The results obtained in nano-scale can be further connected to macro-scale simulation or experiments. Nano-scale solidification allows to obtain various material parameters such as strength and dynamic parameters such as speed of solidification front, hence it is very powerful tool to support macro-scale study. The intention for further research is to combine the nano-scale simulation with continuum models to obtain multi-scale description, which will be much more comprehensive than the usage of empirical models in solidification modelling.

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