

MCGILL UNIVERSITY  
Graduate and Postdoctoral Studies  
**Examiner Report – Master's Thesis**

**Report due date:** August 29, 2017  
**Name of Student:** Nathan Frederick SMITH  
**Degree/Unit:** Master of Science, Department of Physics  
**Thesis title:** Improvements to the binary phase field crystal theory with applications in the kinetics of precipitation

As a thesis examiner, you will complete this form and attach a written report providing a detailed justification of your evaluation. The deadline to send **this form and your written report** to Graduate and Postdoctoral Studies (email: [thesiscoordinator.gps@mcgill.ca](mailto:thesiscoordinator.gps@mcgill.ca)) is **August 29, 2017**. A late report has serious academic and financial consequences for the student. Thank you for your valuable contribution to this student's examination.

**1. Evaluation of the Thesis:** Complete the evaluation grid below and comment on the criteria in your written report.

Criteria for Evaluation of Thesis	Excellent Top 10%	Very Good	Good	Satisfactory	Unsatisfactory
1. Is in line with disciplinary norms	✓				
2. Is situated in a broader context and appropriately acknowledges the larger field of research (e.g., citations/references)	✓				
3. Details methodology and methods	✓				
4. Reports results clearly		✓			
5. Justifies analyses and conclusions		✓			
6. Discusses implications	✓				
7. Is presented appropriately for disciplinary norms (grammar, style, coherence, cohesion)		✓			
8. Complies with McGill's <u>guidelines for thesis preparation</u>	✓				

**2. Overall Recommendation:** Select one.

Recommendation	Select ONE
<b>PASSED</b> – The thesis is <b>ready</b> for final submission. <ul style="list-style-type: none"> <li>Report must include any recommendations for <u>minor</u> revisions to the thesis (i.e., stylistic or editorial changes that can be completed in three weeks or less).</li> </ul>	✓
<b>NOT PASSED</b> – The thesis needs <b>major revisions before resubmitting</b> . <ul style="list-style-type: none"> <li>At least one of the Criteria for the Evaluation of the Thesis must be judged as unsatisfactory if the thesis is NOT PASSED.</li> <li>Report must include a detailed description of the shortcomings that have informed your decision, including an itemized list of substantive issues you would expect the student to address in order for the thesis to be given a PASS.</li> <li>If this is the first NOT PASSED assessment, the student will have the option to <u>revise and resubmit</u> the thesis.</li> </ul>	

DATE : 8/30/2017

SIGNED : Dad Wier  
 (Prof P. W. Wiseman)

## External Reviewers Report of Nathan F. Smith's MSc thesis entitled: Improvements to the Binary Phase Field Crystal Theory with Applications in the Kinetics of Precipitation

This MSc thesis certainly meets the criteria for a master's thesis at McGill University and is very clearly written. After the background introductory chapter, chapters 2, 3 and 4 present a very clear introduction to classical density functional theory (CDFT), application of CDFT to the theory of freezing and phase field crystal (PFC) theory and its variant binary structural PFC (XPFC). These chapters of the thesis contain a very nice review of these methods and present derivations and background with enough detail so that the reader can understand the context of the new extensions to the binary XPFC present in chapter 5 and its application to study dynamics of nucleation in chapter 6. As this thesis includes both a thorough review and new extensions and applications, I feel the author has certainly met the requirements for an MSc thesis as set by the university. It is also one of the best written thesis documents I have reviewed in recent years and I certainly appreciated this as I read the technical theory and results.

For the most part I have only minor grammatical corrections to suggest which are outlined below.

However, I would like the author to justify physical conclusions drawn from Fig. 6.3 on page 65 of the pdf (pg 54 of the thesis). The author quantified the nanoparticle growth simulations from Fig. 6.2 by plotting the mean radius of the solute-rich domains as a function of time, averaging the results over an ensemble of 120 quench simulations. In Fig. 6.3 the author compares the mean radius to that expected for purely diffusive growth (the mean radius scaling linearly with the square root of time for diffusion). The author argues that for early times, there is a hyper-diffusive rate for the growth of crystalline regions and this decays to hypo diffusive growth at longer times after uncrystalline regions have disappeared. This is inferred from the comparison to diffusive growth curves and shown as expanded inset plots.

The slope variations are visually clear from the plot insets but are they statistically robust?

What is the expected error for the plots of the mean radius versus time for an ensemble of 120 simulations and can the deviations from diffusive growth be statistically justified?

I congratulate the author on this excellent work and I feel it is an excellent body of work and definitely a pass.

Minor corrections

Pdf Pg. 4 in the Abstract: phenomenon (singular...phenomena plural...also elsewhere in the thesis

Pdf Pg. 13 (thesis pg. 2) ...and on relatively long timescales, we have the methods of PFC: what is the ballpark order of magnitude for long timescales here?

Pdf Pg. 14 The goal of the current research is threefold: The first two goals

A colon is typically used to introduce an example or a list. I would suggest a stand alone sentence: “The current research has three goals.” The goals can then be introduced in sentences as you have written.

Pdf pg. 16 tractable (not tractible) & intractable (also elsewhere in the thesis).

Pdf pg. 22 after Eq. 2.22 the (not The)

Pdf pg. 24 Eq. 2.28 should be follow by a comma (not a period) and then we notice... (not We)

Pdf pg. 26 above Eq. 2.39 homogeneous (missing the u)

Pdf pg. 32 This phenomenon (not phenomena)

Pdf. pg. 32 critical is repeated

Pdf. pg. 42 above Eq. 4.8: n-c pair correlation[s] introduced...are

Pdf. pg. 46 Temperature dependence of the correlation peaks in the [?] is achieved

In the what?

Pdf. pg. 47 This inhibits the modelling [of] a variety of binary alloy systems,

Pdf. pg. 48 This phenomenon (not phenomena)

Pdf. pg. 48 ...in this th[e]sis which are presented in the following chapter

Pdf. pg. 51 ...in the exact theory that emerges from the original alloy CDFT theory (equation C), we use the labels

What is equation C? Shouldn't this be a numbered equation?

Pdf. pg. 51 after Eqns. 5.6-5.8 a space is needed after generalize

Pdf. pg. 51 Following Greenwood et al[.]

Pdf. pg. 51 The  $\alpha$  and  $\beta$  phase[s] are...

Pdf. pg. 52 above Eq. 5.11 ...choice of interpolation functions: (not interpolations)

Pdf. pg. 53 near the bottom: ...is assumed for each crystal phase (not phases)

Pdf. pg. 56 possible is repeated

Pdf. pg. 57 We first begin with, we introduce a...(grammar)

Pdf. pg. 58 ...changes in composition occur simultaneously [with] changes in order (not to)

Pdf. pg. 59  $n^*$  is the number [of] critical nuclei. (not if)

Pdf. pg. 59 This naïve approach dramatically underestimate[s]

Pdf. pg. 60 ...under certain circumstances indicates that [it] is a metastable liquid...

Pdf. pg. 62 We refer to this [phenomenon] as sacrificial growth...(not phenomena)

Pdf. pg. 64 ...to those shown in figure ?? (figure 6.2?)

Pdf. pg. 64 ...[stages] of growth...(not steges)

Pdf. pg. 64 The data show that...(not shows...data are plural)

Pdf. pg. 66 The is noteworthy that the... (? It is noteworthy that...?)

Pdf. pg. 68 Top line...improper use of the colon.



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Prof. Paul W. Wiseman

August 30, 2017