combined feedback on the paper of Team 1

This document contains the combined feedback of your peers, instructors and a few external people. Everything is anonymized, and there is no guarantee against conflicting opinions. It shows you the impression your paper makes, seen through the eyes of others.

Summarize in one to three lines the main message you got from this paper:

An HCP layer can from on top of an FCC film in case the interface energy between the two phases is negative (or very small positive) and the surface energy of the HCP phase is low enough. However, convergence tests for the vacuum and slab thicknesses, required to study surfaces, are apparently very hard to perform. Whenever they can be executed successfully, one could compute the surface tensions of the separate phases as well as their interfacial tension and from this the maximum HCP top layer could be calculated.

Due to the technical issues this paper didn't provide the desired results. But the paper still provides a theoretical background on how to perform the calculations and some of the criteria that need to be met in order to develop a surface layer. The paper thus provides some kind of pathway that could allow other researchers to obtain the desired results, based on the parameters of the (successful) convergence testing.

It was found in a recent paper that phase separation is present in thin films of Ni80Fe20. In this study, DFT methods are used to replicate the results and the influence of spin-polarized and non-magnetic Ni is evaluated. Also another material is inspected, and a way was sought to determine materials that are likely to show similar behaviour.

The goal of this paper was to use DFT methods to try and replicate the obtained results from a study about the formation of a Ni HCP layer on top of an FCC layer. It is clear that these kind of calculations aren't that straight forward and quite time consuming if convergence is taken to tight.

The goal was to calculate the equilibrium thickness of a HCP Ni phase that formes on a FCC Ni phase in an Ni-sapphire system. For the calculation of surface energy of these phases needed to be found, but due to unkown reasons this was not achieved.

The phase seperation of an FCC bulk and HCP surface within Ni80Fe20 film was calculated via DFT. Convergence for the vacuum thickness to approximate a surface was not acheived, but a theoretical approach was formulated instead.

The quantity that determines whether phase separation occurs in Ni growth on a sapphire substrate is the surface energy between FCC Ni and HCP Ni. It completely determines the behavior of the system.

They wanted to study the growth of FCC and HCP nickel thin films on a sapphire substrate but surface calculations did not converge.

This paper describes the usage of DFT code to study the nickel films (HCP and FCC stacking) on a sapphire substrate. Therefore the authors started off by doing convergence calculations on the materials themselves and then did convergence testing on a nickel surface (generated via supercell

command). After not having non-convergence, the paper proposes that a lower energy per atom would be reached with a thinner film and that the right way to test this would be to make a thickness vs energy plot via the appropriate DFT calculations per thickness.

Trying to replicate the published work of Sharma with DFT. And by doing this, a minimum amount of calculations can be determined to see if the phenomenon occurs. (HCP layers form on top of the film and FCC layers form on top of the substrate)

Via the optimization of surface layers and the minimization of the surface energy it is possible to determine the feasibility to form a certain thin layer system. Further calculations will in turn lead to the determination of the thicknesses of such films. A possibility would be to further extend this research by finding other materials that can form HCP layers on top of FCC bulk material to lower their energy.

After having read a paper, you are usually left with a few questions. Imagine you are lucky to meet an author of the paper you just read at the coffee machine. What are the most pressing questions for clarification you would ask him/her? (at least one, at most three) :

Why is the term \gamma_FH more crucial than the term \gamma_H in inequality 1? I would expect that the surface energy of the HCP phase is equally important to determine the stability of the layered construction, not just the interfacial energy between the HCP and the FCC phase.

"1. Why didn't you test the convergence of HCP for a higher number of vaccuum layers? Because it looks like the last four points (3->6) show some kind of trend.

2. Without performing the required calcuations, do you think that Co would develop a surface layer? Or are there some species where you expect a surface layer? "

"Any clue why the divergence tests were so problematic? Have you tried any further tests?

At page 3, calculations are mensioned to be required but unlikely to be able to be calculated in an appropriate time. How one should then proceed?"

I would like to know the reason why for FCC the (111) and for HCP the (100) surface has been chosen for the surface energies.

You say that adding additional layers in the slab could achieve better results because less noise would be achieved, has such a calculation been done? And what was the result?

The work is based on already performed calculations for the material, were there any differences in approach with the original authors? What could be an application for such films? Why would the addition of Co would have a similar effect?

To me it seems like the results for the surface energy of the HCP and FCC structure would converge just outside the scope of the range you tried. Would it be possible to do these calculations or would this take to much computing time or would this not be physically relevant anymore?

In Fig. 1 which minimal energy value is lower, for FCC or HCP? It is not clear from the picture. Why do you think that "The number of Ni layers must also be tested to make sure that central layers are equivalent to bulk layers."? I think that this is not needed for thin films. Thin films don't have to have

bulk layers. Why Fig.2 does not show results for hcp for more than 6 vacuum layers? FCC looks like converging on Fig.2. Would it converge for non spin polarized calculations (maybe this would give you a hint)? What does Stefaan suggest to do?

What they would do with more time to actually have the surface calculation converge, as they state no possible reasons for this.

Isn't it possible to work further with an average value of the surface energy (obtained by the different number of vacuum layers)?

It turns out that such thin films are theoretically and thermodynamically possible, but are they kinetically feasible in real life and how would the system react if the surface film is damaged for example?

Evaluation on some specific criteria :

	this team (on 10)
the abstract summarizes the main message	4.1
the introduction clearly sketches the context of the research	7.9
the problem is well-described	7.9
where relevant, proper reference to previous work is made	8.1
the methodology is well-described	7.3
the methodology is justified in the text	7.2
the strategy is clearly described and reproducible	6.4
it is clearly described which new results (data) have been obtained	7.1
these data have been interpreted in an understandable and sound way	7.0
the relevance of this work has been pointed out	5.3
the paper conveys excitement and enthousiasm	6.0
global average	6.7

Which advice do you want to give to the authors of this paper ?

"Add an abstract and conclusion to your work, this prepares the reader better to the content and provides him/her a convenient summary at the end to take the most important issues with him/her.

Further, I would suggest them to elaborate a little more on the figures they provided. I really liked the concept of figure 3 (very visual information), but a little more explanation in the text or in the caption would have been welcome. "

"Maybe try to explain why you use certain approximation and criteria. When you lowered the criteria for the surface convergence ("" the energy cut-off values and k-meshes were slightly lower than the agreed convergence criteria"") you didn't mention the new values. I think it's perfectly OK to lower these requirements in order to achieve a higher efficiency, but it might be interesting to provide the new criteria for future reference. "

Don't be demotivated! It is clear you understand the line of research in all of its aspects.

They could have tried other DFT software packages to try to solve their problem regarding the amount of vacuum needed in the supercell.

I can't really think of something

The practical application of the chosen material can be more elaborated. Also, an appendix with the code can be handy to allow other authors to aid in solving the problem.

It seems to me that the surface energies would have converged for more vacuum layers, maybe you could have worked with the largest values you have tried and done the described procedure with these values, keeping in mind that these might be off by a certain percentage.

Check convergence for vacuum for non spin polarized case.

Try to give a part where they explain the methodology in depth rather then just briefly going over the theory and then moving straight to results. Maybe rather than focussing on doing extra research on what needed to be done after the non-converging calculations, try to put more time into simplifying the DFT code until it converges and then work up to a better approximation.

Good paper with a good lay-out! Don't forget to add sources to the equations, otherwise good reference!

It was already good to add a further work section, but it might also be interesting to further hypothesize on those results or what other authors obtained by performing similar calculations.