Towards Phase Field Modelling of Silicon-Gold Eutectic Growth

John Hwang¹, Eric Kueper¹, Zi Wang¹, Kirk H. Bevan¹

¹. Department of Materials Engineering, McGill University, Montreal, QC, H3A 0C5, Canada

Introduction

Growing silicon is usually done vertically aided by a gold catalyst.¹

- Growing silicon horizontally would be more cost effective. Large amount of silicon could be grown quickly for applications in solar panels, semi-conductors, and others.
- However, it is not straightforward to grow silicon horizontally. As show in figure 2 and 3 the silicon is growing in patches and dendrites.
- Use phase field (PF) modelling to understand Au-Si growth process.

Method

- Started by looking at Langevin Simulations of Nonequilibrium Phenomena¹
- Phase field models are usually solved to interfacial problems, mainly applied to solidification dynamics.

Model A

- The non-conserved model: the field is not conserved (one phase can totally change into another phase).
- Model A is generally used to model dynamics of nonequilibrium phenomena such as order-disorder transitions and liquid-solid transitions¹
- Prints an initial field, and then calculates next field through the free energy equation

\[
\frac{d\phi}{dt} = -M(\nabla \phi + \phi \nabla \phi - \kappa \nabla^2 \phi) + \eta.
\]

Model B

- The conserved model: the field is conserved.
- Model B might be better suited for the problem since binary phase separations can only be modelled with the conserved model.²
- For our purposes, we do not want the phases to transition from one to the other phase.
- Difference in coding from model A is an extra Laplacian in the free energy equation.²

\[
\frac{d\phi}{dt} = -M(\nabla \phi + \phi \nabla \phi - \kappa \nabla^2 \phi) + \eta
\]

Model C

- Combination of A and B: there are two fields, the non-conserved phase field and the conserved concentration field.³
- It seems the model C would appear to fit our data better due to the combination of the two fields which produce results that (as shown in figure 6) resemble the growth shown in figure 2 and 3.

Conclusion and Future Work

- Model A does not model the growth well
- Model B matches the growth much better but is still insufficient
- Model C seems to be most suited for the problem. With proper parameters, it should be able to simulate dendrite-like growth as seen in Fig. 2 and 3.
- A better understanding of eutectic Au-Si growth has been achieved by using PF models. This could lead to more efficient production of silicon crystals.
- Model C should be further investigated to model proper growth and the parameters needed for such growth.

References

2 – Ken Elder and Nicolas Provatas, Phase-Field Methods in Material Science and Engineering.

Acknowledgements

This work is supported by the SURE Program and NSERC. We would like to thank Jerome Leboeuf for the data provided and for assisting with the project.

John Hwang
Department of Mining and Materials Engineering
6810 Rue University, Montreal, Quebec, H3A 0C5
Email: jhy1030@hotmail.com

McGill University