TUE/E3.1
15:30–15:50

Macroscopic diffusion models for precipitation in crystalline gallium arsenide

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Based on a thermodynamically consistent model for precipitation in gallium arsenide crystals including surface tension and bulk stresses by Dreyer and Duderstadt [1], we propose different mathematical models to describe the size evolution of arsenic-rich liquid droplets in crystalline gallium arsenide [2]. These models generalise the well-known Mullins-Sekerka model for Ostwald ripening. Droplets can shrink or grow with time but the centres of droplets remain fixed. The outer boundary of the domain is also a free boundary.
Some of the models lead to a quasilinear parabolic PDE for the chemical potential, which is coupled to an elliptic boundary value problem for the displacement and to ODEs for the free boundaries. Due to different scales for typical distances between droplets and typical radii of liquid droplets we can reduce formally this problem to a large system of ODEs coupled by a mean field, so-called mean field models. For one of the models we prove the mean field model in the limit of small volume fraction by homogenisation techniques under plausible assumptions [2]. These mean field models generalise the Lifshitz-Slyozov-Wagner model, which can be derived from the Mullins-Sekerka model rigorously [3].
Mean field models capture the main properties of our system and are well adapted for numerics and stability analysis. Numerical evidence suggests in which case which one of the models might be appropriate to the experimental situation [2].

[1] W. DREYER, F. DUDERSTADT: On the modelling of semi-insulating GaAs including surface tension and bulk stresses. *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.*, **464** (2008), 2693–2720.

[2] S.-J. KIMMERLE: Macroscopic diffusion models for precipitation in crystalline gallium arsenide – Modelling, analysis and simulation. *PhD thesis, HU Berlin* (2009), submitted.

[3] B. NIETHAMMER: Derivation of the LSW-theory for Ostwald ripening by homogenization methods. *Arch. Rational Mech. Anal.*, **147** (1999), 119 – 178.