Simulation of Liquid Film Migration

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ABSTRACT

A model is proposed describing the movement of a thin liquid film in a crystal. The model describes two sharp solid/liquid interfaces (leading melting interface and trailing solidifying interface) that migrate simultaneously. Considering recent experimental results on grain boundary melting and segmentation of liquid films at former grain boundaries, the driving force for migration could be better identified. Driving forces suggested in the literature such as coherency strains can be excluded to be responsible for the migration.

In the present case, migration is driven by slight deviations from local equilibrium e.g. due to temperature changes at the interface. The initial migration direction of the film is set by temperature fluctuations. In the model, the driving forces are determined by means of an interface thermodynamics model. An extended mass balance equation taking into account the fluxes in the adjacent phases at both interfaces of the thin film is introduced. The mass balance together with the diffusion fluxes accounts for the interaction between the two migrating interfaces. It is necessary to consider the above mentioned slight deviations from local equilibrium even for low interface velocities, as local equilibrium models will necessarily predict immobile liquid films. Supersaturations in the order of 0.01% to 0.001% are calculated to be sufficient for film migration velocities from mm/s to µm/s.

Simulation results are compared with experimental findings, good (semi-quantitative) agreement with own and published data on migrating liquid films is achieved.