The prediction of structure evolution in Al-Si using phase field modeling method

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We present a theoretical study on the prediction of the structure evolution in system Al-Si. The calculations were performed using the phase field modelling method and the Moose software [1]. The applied Kim-Kim-Suzuki (KKS) model is a two-phase model (with a single order parameter η) with the added complexity, which is done by introducing phase-concentrations to both phases [2]. The complementary calculations were performed using Thermo-Calc software [3].

The construction of the model plays a crucial role in the studying of the structure evolution by the phase field modelling method. Here, tree models for different temperatures were built. The initial structure was read from the SEM images provided by Kim Vanmeensel group. The composition, mobility and the description of the free energy evolution with respect to the temperature and composition were determined using the Al-Mg COST 507 thermochemical database for light metal alloys [4].

The number, volume and shape of the precipitates was observed with respect to the changing temperature and time of the evolution. The initial structure consisted mainly of the matrix fcc aluminium phase. During the evolution, the small precipitates with diamond structure (consisting mainly of silicon) were growing and forming spherical shapes. The theoretical results were compared with the experimental ones provided by the group of Kim Vanmeensel.

[1] Gaston D.R., Permann C.J., Peterson J.W., Slaughter A.E., Andrš D., Wang Y., Short M.P., Perez D.M., Tonks M.R., Ortensi J., Martineau R.C., Ann Nuclear Energy, 84 (2015) 45–54. Special Issue on Multi-Physics Modelling of LWR Static and Transient Behaviour. https://doi.org/10.1016/j.anucene.2014.09.060.
[2] Kim et al., Phys. Rev. E, 60 (1999) 7186-7197.
[3] Andersson J.O., Helander T., Höglund L., Shi P.F., Sundman B., Calphad, 26 (2002) 273-312.
[4] Ansara I., Dinsdale A.T., Rand M.H., ed.: COST 507. Definition of Thermophysical Properties to Provide a Database for the Development of New Light Alloys. Thermochemical Database for Light Metal Alloys. Vol. 2., Scientific Group Thermodata Europe Database, EUR 18499 en (1998).