Investigation of the Grain-Boundary Segregation Transition in the Binary Fe-C Alloy

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Abstract : Grain boundary segregation transition (GBST) has been calculated by a thermodynamic model in binary alloys. The method is used on cementite (Fe3C) segregation in base-centered cubic (ferrite) iron (Fe) in the Fe-C binary system. The GBST line is shown in the Fe3C lacking part of the phase diagram with high solvent (Fe) concentration. At a lower solute content (C) or at higher temperature the grain boundary is composed mostly of the solvent atoms (Fe). On higher concentration compared to the GBST line or at lower temperature a phase transformation occurs at the grain boundary, the latter mostly composed of the associates (Fe3C). These low-segregation and high-segregation states are first order interfacial phase transitions of the grain boundary and can be transformed into each other reversibly. These occur when the GBST line is crossed by changing the bulk composition or temperature.

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