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Modeling Solute Segregation during the Solidification of γ-phase U-Mo Alloys

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Using first principles calculations, it is demonstrated that solute segregation during U-Mo solidification can be modeled using the classic Brody-Fleming limited diffusion framework. The necessary supporting equations specific to the U-Mo alloy, along with careful verification of the assumptions underpinning the Brody-Fleming model are developed, allowing for concentration profile predictions as a function of alloy composition and cooling rate. The resulting model is compared to an experimental solute concentration profiles, showing excellent agreement. Combined with complementary modeling of dendritic feature sizes, the solute segregation model can be used to predict the complete microstructural state of individual U-Mo volume elements based upon cooling rates, informing ideal processing routes.

Keywords: U-Mo Alloys, Solute Segregation, Brody-Fleming Model

Introduction

A fundamental scientific concern during the processing of U-Mo alloys is their susceptibility to solute segregation during solidification, typically producing a microstructure of Mo-rich dendrites [1]. This can pose significant technical problems as it is often desirable to quench in the high-temperature body centered cubic (bcc) γ-phase of the U-Mo system, preserving both microstructural uniformity and the isotropic material properties associated with cubic phases. Under equilibrium conditions the U-Mo system experiences a eutectoid decomposition below ~570°C from the solidified γ-phase into the non-cubic α and γ' phases [2] [3]. The orthorhombic α-phase is particularly detrimental to the mechanical stability of the alloy due to its unique anisotropic properties, including a negative thermal expansion coefficient along one crystallographic direction [4]. Transformation kinetics through the low-temperature