OC-17 PHASE-FIELD MODELLING OF GLASS CRYSTALLIZATION: CHANGE OF THE TRANSPORT PROPERTIES AND CRYSTALLIZATION KINETICS

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The viscosity of a supercooled liquid changes several orders of magnitude near the glass transition temperature T_g. In this supercooled region, either temperature or compositional changes are expected to induce large variations of the viscosity and hence of the atomic transport properties of the glass. Primary crystallization occurs in a deeply undercooled liquid in metallic glasses. In many cases the crystallization temperature T_x is not far over T_g. The compositional changes of the glassy matrix during primary crystallization are then expected to influence the atomic transport properties and hence the crystallization kinetics.

Understanding primary crystallization kinetics is a key point in controlling microstructural development of partially crystallized metallic glasses. Some kinetic models describe primary crystallization by means of a mean-field reduction of the crystalline growth rate as the transformation proceeds [1,2]. Such a reduction is commonly associated with a decrease of the concentration gradient surrounding the crystallites due to the overlap of the neighbouring particles concentration fields (soft impingement). However, these models do not seem to be able to fully explain the kinetic behaviour of such transformations. Moreover, the slowing down of the structural relaxation dynamics due to the composition change is expected to influence significantly the crystallite growth rate. The estimation of such effect would improve the description of the crystallization kinetics.

In this work we perform many-particle phase-field simulations of primary crystallization with a coefficient of diffusion dependent on the local composition of the untransformed matrix. The results show that the experimental kinetics observed in primary crystallization of many metallic systems can not be described by the soft-impingement effect but to the change of the transport properties of the matrix as the transformation proceeds.

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