Fast Crystal Growth: analysis of field and atomistic data of simulation

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A summary of atomistic data of simulation on growth kinetics of elemental (Fe, Ni, Al, Cr, Si) and binary (AlNi, CuZr, SiAs) crystals is presented. An analysis of the data is given using kinetic theories of crystals growth for various crystallographic orientations, especially, diffusion-limited theory [1,2], collision-limited theory [3,4], and density-wave theory [5]. Particularly, it is shown that the results of atomistic simulations of the crystallization process reveal a complex temperature dependence of the velocity of the crystal–liquid interface featuring an increase up to a maximum at 10–30% undercooling below the equilibrium melting temperature followed by a gradual decrease of the velocity at deeper levels of undercooling. At the qualitative level, such non-monotonous behavior of the crystallization front velocity is consistent with the kinetic theories [1-5], where the almost linear increase of the interface velocity in the vicinity of melting temperature is defined by the growth of the thermodynamic driving force for the phase transformation, while the decrease in atomic mobility with further increase of the undercooling drives the velocity though the maximum and into a gradual decrease at lower temperatures. At the quantitative level, however, the kinetic theories fail to describe the results of atomistic simulations in the whole range of temperatures with a single set of parameters for some of the model materials.

To describe crystal-liquid interface propagation in a widest range of temperatures the predictions of the kinetic phase field model [6] formulated for small and large driving forces on solidification and melting is used. These predictions were made using traveling wave solutions of the phase field equation describing non-linear behavior in the kinetic crossover from slow to fast mode of the crystal-liquid interface propagation. The described kinetic effects are included in the dendrite growth model [7] whose predictions are compared with experimental data on the rapid dendritic solidification of binary alloys. It is shown that the transition from crystal to glass formation is accompanied by the abrupt-drop in the interface velocity at highest undercooling.

References

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