Two-temperature modeling of crystal growth in supercooled melt

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The two-temperature model (TTM) coupled to molecular dynamics (MD) simulation [1, 2] is used to study crystal-growth rate of tungsten into a supercooled melt in a quasi-one-dimensional case. To simulate heat dissipation into the surrounding medium, heat sinks are added at the boundaries of the electronic subsystem [3]. The heat sinks provide a more realistic description of the electronic thermal transport away from the system compared to periodic boundaries for the electronic subsystem, allowing us to account for the heat dissipation from the crystallization front. Comparisons are established with respect to MD and standard TTM simulations. We have found that the temperature and the value of the maximum growth rate are the same regardless of whether TTM simulations are used. In contrast, the inclusion of sinks has a great impact on the crystal growth rates at the temperatures away from the fastest-growth temperature. At low temperatures, a frustration of the liquid–crystal interface dynamics is seen until a state of zero crystal growth is reached with a stable boundary between crystal and amorphous phases [4].

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