

Melting of ideal and real materials

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The nature of melting transition is not yet fully understood. Significant effort is dedicated to studies of melting by molecular dynamics simulation. A special effort has to be made to melt a perfect crystal at the thermodynamic melting point without superheating in these simulations. On the contrary, real materials melt readily at the melting point and a special effort is required to heat them above the melting temperature. Several explanations have been suggested for such a difference between melting of ideal and real materials. By investigating the impact of defects, grain boundaries and grain junctions, we conclude that the melting in real materials is initiated at the grain junctions. Correspondingly, to superheat a real material it has to be a single crystal to eliminate the impact of the junctions and to be embedded in the crystal with much higher atomic weight to avoid premelting.