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.