Table of Contents

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Structure of the Solid-Liquid Interface

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Theoretical works on the structure and thermodynamic properties of the solid-liquid interface of a simple substance are reviewed. The methods of investigation follow those which have been applied in the case of the bulk liquids: Bernal random packing of hard sheres, computer simulations and perturbation theory. Application of these techniques allows a description of the interface, in terms of density profile and structure of the interfacial layers. The interfacial specific free energy is estimated in the case of the (111) fcc orientation.

Future developments will tend to the calculation of the interfacial free energy in different directions, as well as to a better understanding of the phenomena which occur at the interface during growth of a crystal from the melt.

Crystals 9
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