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Physics Reports 411 (2005) 291–321
PHYSICS REPORTS
www.elsevier.com/locate/physrep

# Melting and nonmelting of solid surfaces and nanosystems

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Accepted 31 January 2005
Available online 7 April 2005
editor: G. Comsa

**Abstract**

We present an extensive but concise review of our present understanding, largely based on theory and simulation work from our group, on the equilibrium behavior of solid surfaces and nanosystems close to the bulk melting point. In the first part we define phenomena, in particular surface melting and nonmelting, and review some related theoretical approaches, from heuristic theories to computer simulation. In the second part we describe the surface melting/nonmelting behavior of several different classes of solids, ranging from van der Waals crystals, to valence semiconductors, to ionic crystals and metals. In the third part, we address special cases such as strained solids, the defreezing of glass surfaces, and rotational surface melting. Next, we digress briefly to surface layering of a liquid metal, possibly leading to solid-like or hexatic two-dimensional phases floating on the liquid. In the final part, the relationship of surface melting to the premelting of nanoclusters and nanowires is reviewed.
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*PACS:* 61.30.Hn; 64.70.Dv; 68.08.−p; 68.35.Md; 61.46.+w

*Keywords:* Surface melting; Surface phase transitions; Surface thermodynamics; Wetting; Molecular dynamics simulation

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doi:10.1016/j.physrep.2005.01.004

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## 1. Introduction: surface melting/nonmelting

Melting, certainly one of the longest known phase transitions, always appeared a very special one. Although undoubtedly first order, it curiously displays only *half* the hysteresis cycle one would expect. In a regular first-order phase transition, the free energies of two phases cross, while both remain locally stable beyond the crossing. As a result, it is generally possible to undercool the high-temperature phase, and to overheat the low-temperature phase. Periodic heating and cooling through a first-order transition will thus generate a full hysteresis cycle.

In melting, this is only half true. It is generally possible and easy to supercool a liquid: a glass of water may not freeze at all during an icy night, only to do that suddenly when disturbed the next morning. On the contrary, it is surprisingly difficult and often impossible to overheat a free solid. The reason for that is that a free solid has surfaces; and when the melting temperature is approached, melting of the bulk crystal is ready to begin from there. Supercooling of the liquid is allowed by the absence of a solid germ; overheating of the solid is prevented by that omnipresent germ, a wet surface. This observation provides perhaps the first macroscopic hint that solid surfaces might be wet already somewhat below the melting point. The starting motivation for a microscopic study of surface melting begins right there.

Consider a semi-infinite homogeneous solid, e.g., a crystal with a free surface, in thermodynamic equilibrium at temperature $T$ and pressure $P$ with its own vapor (Fig. 1). As $T$ and $P$ are raised to approach melting at the bulk triple point ($T_m$, $P_m$), where solid, gas and liquid coexist, the solid–vapor interface will generally wet itself with an atomically thin liquid film, whose thickness $\ell(T) \to \infty$ when $T \to T_m$. This is called surface melting (SM). A rather famous microscopic characterization of SM is that of Pb(1 1 0), first reported by Frenken and van der Veen [1]. Medium energy ion scattering data reveal (Fig. 2) the

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