Zeitschrift: Helvetica Physica Acta
Band: 62 (1989)
Heft: 6-7

Artikel: Surface supermelting with long-range potential

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DOI: https://doi.org/10.5169/seals-116115

SURFACE SUPERMELTING WITH LONG-RANGE POTENTIAL

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Abstract: A system of long-range potential with the tail of r^{-4} is studied, both by mean-field theory and molecular dynamics simulations. The expected cross-over from a "slow", logarithmic-like thickness growth at low temperatures to a "fast", power-law growth closer to the triple point is found to occur. In the power-law growth regime the exponent is $\simeq 1$ in agreement with the predictions of phenomenological theory. The absolute film thickness, however, is severely underestimated by mean-field theory.

Recently it was demonstrated that the surface melting depends crucially upon the long-range behavior of the interatomic potential [1,2]. For some crystals, potentials more long-ranged then Lennard-Jones (LJ) are expected, for example, when the dipole-dipole and quadrupole interactions are important. The effect of turning the potential into more attractive is to favor the denser phases, and thus it makes the quasi-liquid layer thicker. Moreover, such potential suppresses the fluctuations additionally and therefore a theory, based on the mean-field (MF) approximation should be more accurate.

Molecular dynamics (MD) has not been successful so far in describing surface melting since the temperature cannot approach very closely the triple point. However, when enhanced surface melting occurs (as in the case of long-range potentials), MD studies should become feasible and hopefully bring useful information.

Here we present the results of both MD and MF theory [3] of a system with a model potential which coincides with the LJ potential inside the range $r_0 = 3.2\sigma$ and it is continued with a tail $\sim r^{-4}$. The long-ranged attraction gives rise, as expected, to an enhanced thickness of the quasi-liquid layer in comparison with the LJ surface. The results of the MF theory agree well with the MD simulation. A crossover from a "slow", logarithmic-like thickness growth at low temperatures to a "fast", power-law growth closer to the triple point is found to occur (see figure 1). In the power-law regime the exponent is ≈ 1 in agreement with the predictions of the phenomenological theory [4]. However, the real thickness of the liquid film, as extracted from MD is ~ 5 times larger than that found by MF. Hence fluctuations appear to be still quite important.

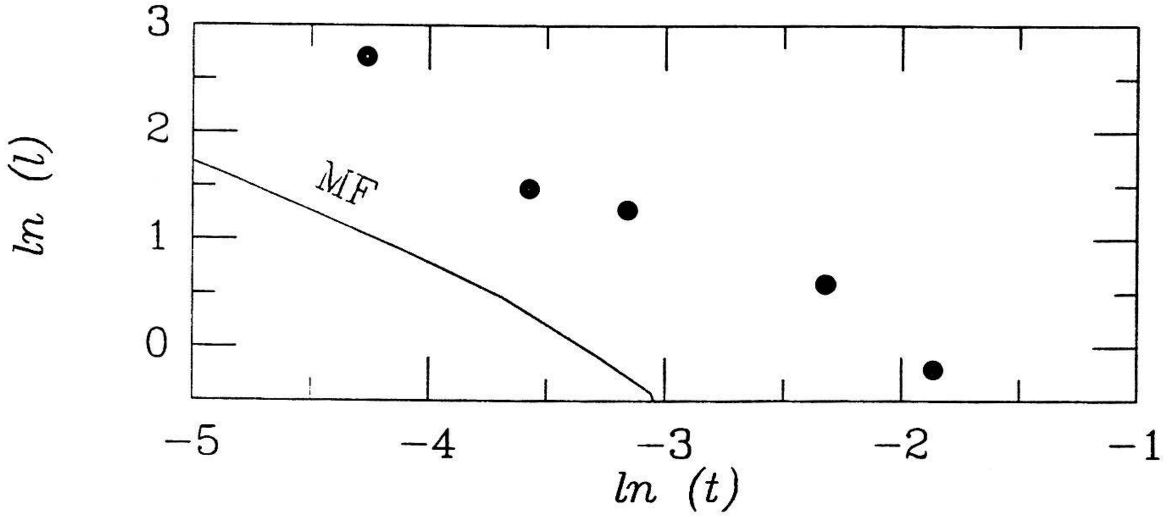

Figure 1: Log-log plot of the molten layer thickness versus normalized temperature $t = \frac{T_m - T}{T_m}$. The dots are molecular dynamics results. Solid line is produced by mean-field theory. Both the molecular dynamics and mean-field theory give the growth exponent to $\simeq -1$. The absolute film thickness, however, is severely underestimated by mean-field theory. In MD, $T_m \simeq 0.71$.

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