

Surface supermelting with long-range potential

Autor(en): **Chen, X.J. / Ercolessi, F. / Tosatti, E.**

Objekttyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **62 (1989)**

Heft 6-7

PDF erstellt am: **26.04.2024**

Persistenter Link: <https://doi.org/10.5169/seals-116115>

Nutzungsbedingungen

Die ETH-Bibliothek ist Anbieterin der digitalisierten Zeitschriften. Sie besitzt keine Urheberrechte an den Inhalten der Zeitschriften. Die Rechte liegen in der Regel bei den Herausgebern.

Die auf der Plattform e-periodica veröffentlichten Dokumente stehen für nicht-kommerzielle Zwecke in Lehre und Forschung sowie für die private Nutzung frei zur Verfügung. Einzelne Dateien oder Ausdrucke aus diesem Angebot können zusammen mit diesen Nutzungsbedingungen und den korrekten Herkunftsbezeichnungen weitergegeben werden.

Das Veröffentlichen von Bildern in Print- und Online-Publikationen ist nur mit vorheriger Genehmigung der Rechteinhaber erlaubt. Die systematische Speicherung von Teilen des elektronischen Angebots auf anderen Servern bedarf ebenfalls des schriftlichen Einverständnisses der Rechteinhaber.

Haftungsausschluss

Alle Angaben erfolgen ohne Gewähr für Vollständigkeit oder Richtigkeit. Es wird keine Haftung übernommen für Schäden durch die Verwendung von Informationen aus diesem Online-Angebot oder durch das Fehlen von Informationen. Dies gilt auch für Inhalte Dritter, die über dieses Angebot zugänglich sind.

SURFACE SUPERMELTING WITH LONG-RANGE POTENTIAL

X. J. Chen, F. Ercolessi, E. Tosatti and A. Trayanov

International School for Advanced Studies, Trieste, Italy

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 than 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.

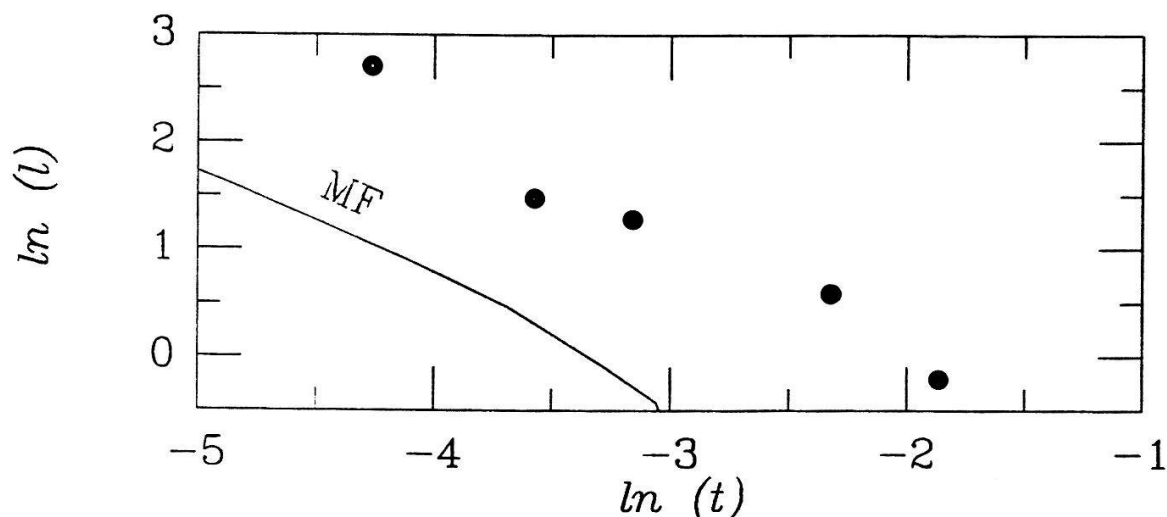


Figure 1: Log-log plot of the molten layer thickness versus normalized temperature $t = \frac{T_m - T}{T_m}$. The dots are molecular dynamics results. Solid line is produced by mean-field theory. Both the molecular dynamics and mean-field theory give the growth exponent to $\simeq -1$. The absolute film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

References

- [1] E. Tosatti and A. Trayanov, *Phys. Rev. Lett.* **59**, 2207 (1987)
- [2] B. PLuis, T. N. Taylor, D. Frenkel and J. F. van der Veen, to appear in *Phys. Rev. Lett.* (1989)
- [3] E. Tosatti and A. Trayanov, Preprint (1989)
- [4] S. Dietrich, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. Lebowitz (Academic, London, 1987), vol. 12