Appunti di Fisica '09

15 gennaio ore 15.30, aula A
Dip. di Fisica della Materia e Ingegneria Elettronica

Anomalous melting behavior under extreme conditions: hard matter turning "soft"

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Standard melting behavior is currently assumed to consist in a regularly increasing and concave melting curve $T_m(P)$. This behavior is exhibited, at least at low pressures, by most substances and is typical of system models such as, e.g., hard-sphere and inverse-power potentials. However, for a number of substances it has been found that at high pressures $T_m(P)$ passes through a maximum followed by a region of re-entrant melting after which, upon further pressure increasing, the melting line may recover a positive slope again (e.g. Cs, K, Na, Ba, Sr, etc.). Melting with non-standard features, including re-entrant melting, is of interest also in a completely different context, that of soft matter, where it has been observed in systems such as star polymers and charged microgels.

We show, through numerical simulation, that a system of particles interacting through the exp-6 pair potential, commonly used to describe effective interatomic forces under high compression, exhibits anomalous melting features such as re-entrant melting and a rich solid polymorphism, including a stable BC8 crystal. We relate this behavior to the crossover, with increasing pressure, between two different regimes of local order that are associated with the two repulsive length scales of the potential. Our results provide a unifying picture for the high-pressure melting anomalies observed in many elements and point out that, under extreme conditions, atomic systems may reveal surprising similarities with soft matter.