Phase behaviour and inverse melting in a water-inspired model

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ABSTRACT: We employ several computer simulation techniques to study the phase behaviour of a simple, two dimensional monodisperse system of particles interacting through a core-softened potential comprising a repulsive shoulder and an attractive square well. This model was previously constructed and used to explore anomalous liquid behaviour in 2D and 3D, including liquid-liquid phase separation [1]. The calculated phase diagram includes six crystal phases in addition to the liquid and gas. Interestingly, we find that one of the melting curves exhibits inverse melting, for which the liquid freezes to a crystal upon isobaric heating over a very small range of pressure [2]. We find that the range of inverse melting can be enlarged by increasing the extent of the repulsive shoulder, and show that despite occurring in 2D, the melting transition is first order and to a liquid, rather than to a hexatic or quasicrystal phase [3]. As this range increases, the topology of the phase diagram changes systematically until it breaks, leading to even more crystal phases appearing.

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