

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Interfacial free energy and stiffness of the solid-melt interface of NaCl TATYANA ZYKOVA-TIMAN, Chemistry Department, Cambridge Uni, ERIO TOSATTI, SISSA-ISAS, International School for Advanced Studies, DAAN FRENKEL, Chemistry Department, Cambridge Uni — The importance of the interfacial free energy for the equilibrium morphology of crystals is well understood. In contrast, much less is known about the so-called “interfacial stiffness” that governs fluctuations of, e.g., solid-liquid interfaces. We carried out molecular dynamics simulations of capillary wave fluctuations on various faces of NaCl crystals in contact with its melt, that provides new information on the behaviour of this interface at the atomistic level. The capillary fluctuations connect directly with the interfacial stiffness, and indirectly also to the interface free energy. In our simulations we studied the (100)-liquid interface and adjacent vicinals. From the angular dependence of the surface stiffness, we deduce an estimate of NaCl(100)-melt interfacial free energy and discuss limitations of the fluctuation approach. Finally we compare this estimate of the surface free energy with values obtained through other methods [1,2,3] and discuss the differences [4].

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Date submitted: 12 Nov 2010

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