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INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

Special Seminar

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joint work with: [1]**S. Angioletti-Uberti,** [3]**M. Ceriotti and** [1]**P.D. Lee**
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ICAMS Seminar room UHW 11/1102

The crystal-melt interface free energy from metadynamics

The solid-liquid interface free energy is a key parameter controlling nucleation and growth during solidification, as well as the energetics of wetting. It is difficult to obtain experimentally, and although there are computational approaches with atomistic simulation, they are difficult to apply routinely. We propose a new approach [1], which is to obtain a free energy map of the phase transition by metadynamics [2]. We have applied this to the benchmark case of a Lennard-Jones potential and the results confirm the most reliable data obtained previously. Our approach offers several advantages: it is simple to implement, robust and free of hysteresis problems, it provides a rigorous and unbiased estimate of the statistical uncertainty and a good estimate of the thermodynamic limit, with system sizes of a just a few hundred atoms. It is therefore attractive for using with more realistic and specific models of interatomic forces.

1 S. Angioletti-Uberti, M. Ceriotti, M.W. Finnis and P.D. Lee, Solid-Liquid Interfacial Free Energy from Metadynamics simulations, Phys. Rev. B, to be published

2 A. Laio and M. Parrinello, Escaping free energy minima, Proc. Natl. Acad. Sci. USA 99: 12562-12566 (2002)