Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

**Fundamental measure density functional theory study of hard spheres solid-liquid interface** VADIM WARSHAVSKY, XUEYU SONG, Department of Chemistry and Ames Laboratory, Iowa State University, Ames, IA 50011 — Interfacial free energy is an important characteristic of solid-liquid interface as it is one of the crucial parameters in many formula of interface thermodynamics such the nucleation theory. Previously different aspects of crystal-melt interfaces were intensively studied with simulations [1,2,3], but theoretical studies with Density Functional Theories (DFT) are inconclusive [4,5]. In this report the structure of hard spheres fcc crystal-melt interfaces and the anisotropy of the interfacial free energies are studied using the Rosenfeld's Fundamental Measure DFT as such a functional leads to reliable coexistence results not only for the hard sphere system but also for the Lennard-Jones systems [6]. The parameters of interfacial density profile were calculated by a proper minimization procedure. For the equilibrium density profile the interfacial free energies were compared with simulation results. 1. R.L.Davidchak and B.B.Laird, Phys.Rev.Lett., 85, 4751(2000). 2. J.J. Hoyt, M. Asta and A. Karma, Phys.Rev.Lett., 86, 5530 (2001). 3. J.R.Morris and X.Song, J.Chem.Phys., 119, 3920 (2003). 4. W.A.Curtin, Phys.Rev.B, 39, 6775(1989). 5. R.Ohnesorge, H.Lowen, and H.Wagner, Phys.Rev.E, 50, 4801 (1994). 6. V.Warshavsky and X.Song, Phys.Rev.E, 69, 061113 (2004).

Vadim Warshavsky
Department of Chemistry and Ames Laboratory, Iowa State University
Ames, IA50011

Date submitted: 15 Dec 2004 Electronic form version 1.4