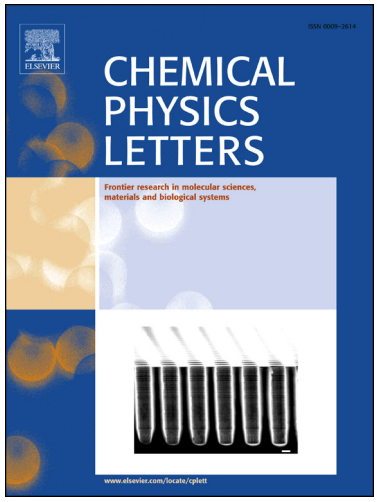

Research paper

Surface free energy and some other properties of a crystal–vapor interface: Molecular dynamics simulation of a Lennard-Jones system

V.G. Baidakov, A.O. Tipeev, K.R. Protsenko

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SURFACE FREE ENERGY AND SOME OTHER PROPERTIES OF A CRYSTAL–VAPOR INTERFACE:

Molecular dynamics simulation of a Lennard-Jones system

V.G. Baidakov *, A.O. Tipeev, K.R. Protsenko

Institute of Thermal Physics, Ural Branch of the Russian Academy of Sciences, Amundsen street 107a, Ekaterinburg, 620016, Russia

Abstract

The surface tension γ and surface energy $\overline{u}$ have been calculated in molecular dynamics simulation of an FCC crystal-vapor equilibrium in systems containing from 54000 to 108000 Lennard-Jones (LJ) particles with a cutoff radius of the potential $r_c = 6.78d$. The surface entropy $\overline{s}$ and the surface free energy σ along the sublimation line have been determined by the method of thermodynamic integration from the zero of temperature, where the classical entropy has been obtained from the dynamical theory of crystal lattice by data on $\gamma(T)$ and $\overline{u}(T)$. Calculations were made on the planes (100), (110) and (111) of an LJ crystal. The anisotropy of surface properties is considerable at low temperatures and smooths over at the approach of the triple point. At a temperature 1/3 lower than the melting temperature of the bulk phase changes are observed in the character of temperature dependences of the properties of a crystal-vapor interface, which are connected with surface premelting. The temperature of the beginning of surface premelting correlates with that at which the metastable extension of the melting line meets the spinodal of a stretched liquid.

* Corresponding author.

E-mail address: baidakov@itp.uran.ru (V.G. Baidakov).