Adhesion Energy, Surface Traction and Surface Tension in Fe-Mg Binary Alloys

Gboyega A. Adebayo[a,b] and Bede C. Anusionwu[a,c]

[a] International Centre for Theoretical Physics, Strada Costiera 11, P.O. Box 586, I-34014 Trieste, Italy
[b] Department of Physics, University of Agriculture, PMB 2240, Abeokuta, Nigeria
[c] Department of Physics, Federal University of Technology, Owerri, Nigeria

Reprint requests to G. A. A.; E-mail: gadebayo@ictp.it

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We present adhesion and surface energies of Fe-Mg binary alloys from simulation studies. The adhesion energy was calculated using the assumption that work is done when atoms come into contact by moving two surfaces from equilibrium position z_o to ∞, while the surface traction was determined from the atomic interactions between atoms. The surface tension variation with temperature was investigated from the diffusion coefficient obtained by performing molecular dynamics simulations at temperatures above the eutetic temperature of Fe-Mg. It was observed that the structural information as well as the calculated surface tension suggest segregation in Fe-Mg alloys at all investigated temperatures.

Key words: Self-Diffusion Coefficient; Binary Alloys; Viscosity; Lennard-Jones Potential.
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