Surface segregation energies in transition-metal alloys

We present a database of 24 x 24 surface segregation energies of single transition metal impurities in transition-metal hosts obtained by a Green's-function linear-muffin-tin-orbitals method in conjunction with the coherent potential and atomic sphere approximations including a multipole correction to the electrostatic potential and energy. We use the database to establish the major factors which govern surface segregation in transition metal alloys. We find that the calculated trends are well described by Friedel's rectangular state density model and that the few but significant deviations from the simple trends are caused by crystal structure effects. [S0163-1829(99)05424-7].