First-principles solution to the problem of Mo lattice stability
IGOR ABRIKOSOV, CHRISTIAN ASKER, ARKADY MIKHAYLUSHKIN, Department of Physics, Chemistry and Biology, Linkoping University, Sweden, ANATOLY BELONOSHKO, Applied Materials Physics, The Royal Institute of Technology, Sweden — The energy differences between the ground state body-centred structure (bcc) and closed-packed face-centred structure (fcc) structures for transition metals in the middle of the series show unusually large disagreements when they are obtained by the thermochemical approach based on the analysis of experimental data or by first-principles electronic structure calculations. Considering a typical example, the lattice stability of Mo, we present a solution to this long-standing problem. In contrast to conventional total energy calculations within Density Functional Theory framework, we carry out ab initio molecular dynamics simulations for the two phases at high temperature. We show that at these conditions both bcc and fcc structures of Mo are dynamically stable, and the difference in their configurational energies decreases dramatically as compared to the zero temperature result, approaching the value derived by means of the thermochemical approach. We show that the main contribution to the effect comes from the modification of the canonical band structure for bcc and fcc phases due to lattice vibrations at high temperature, and discuss consequences of our finding for future first-principles simulations of phase stability.

Igor Abrikosov
Department of Physics, Chemistry and Biology, Linkoping University, Sweden

Date submitted: 26 Nov 2007				Electronic form version 1.4