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Ab initio studies of magnetism at extreme volume and shape deformation MOJMIR SOB, Masaryk University, Brno, MARTIN FRIAK, Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, DOMINIK LEGUT, Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, MIROSLAV CAK, Faculty of Mechanical Engineering, Brno University of Technology, MARTIN ZELENY, Faculty of Chemistry, Brno University of Technology — Magnetic solids constitute a basis of many technologically important materials, however, very little is known how their magnetic behavior changes when a high-strain deformation is applied (as it is, for example, in heavily deformed regions of extended defects, such as grain boundaries, dislocation cores, crack tips etc.). In the present talk, we report on magnetic behavior of iron, nickel, FeCo, Ni_3Al and Fe_3Al at the extreme volume as well as tetragonal and trigonal deformation. The total energies are calculated by spin-polarized full-potential LAPW method and are displayed in contour plots as functions of tetragonal or trigonal distortion c/a and volume; borderlines between various magnetic phases are shown. Stability of tetragonal magnetic phases of γ-Fe is discussed. In case of Fe, Ni and FeCo, the calculated phase boundaries are used to predict the lattice parameters and magnetic states of overlayers from these materials on various (001) substrates. Whereas magnetism does not play an important role in stabilization of the $L1_2$ structure in Ni_3Al, the magnetic effects in Fe and Fe_3Al are vital.

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