

Structure and lattice dynamics of low periodicity Fe_m/Au_n multilayers.

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Although a technological progress in preparation methods of magnetic films enables the possibility to grow the Fe_m/Au_n structures with the thickness down to one monolayer, the formation of low periodicity Fe_m/Au_n multilayers is still problematic.

Using the first principle methods we have found several Fe_m/Au_n ($m, n < 4$) structures with minimal ground-state energy and we have calculated the phonon dispersion relations, and the phonon density of states spectra for them. For multilayers with single Fe or Au monolayer the imaginary vibration frequencies (soft modes), which characterize the unstable structures, were found. To get the stable configuration the additional relaxation of atomic positions, which in consequence can change the space group and the volume of primitive cell, was required. The search of new stable configuration was carried out using the displacement pattern corresponding to the frozen soft phonon mode. The multilayers with thicker Fe layers are stable, since they possess only positive vibration frequencies.

The calculated phonon density of state spectra showed to be very sensitive to the multilayer structures, as exemplified in figure below:

