Self-Organization of Co Atoms Embedded Into the First Layer of a Cu(100) Surface

Kolesnikov S.V., Klavsyuk A.L., Saletsky A.M.

Lomonosov Moscow State University,
Leninskie Gory, Moscow, 119992, Russian Federation
E-mail: kolesnikov_s_v@mail.ru

Magnetic nanostructures are appealing for development of nanotechnology and, in particular, for engineering of nanocomputers. Nowadays several ways of creating such structures are known, however, the simplest way is self-organization. The self-organization of various types of nanostructures on metal surfaces is reported in plenty of experimental and theoretical articles. Unfortunately, not every of such nanostructures are stable at room temperature because of the high mobility of alloy’s atoms. At the same time, alloy’s atoms embedded into the first layer of the metal substrate are immobile at room temperature and can be used for creation of stable nanostructures [1,2].

We present the theoretical investigation of the self-organization of Co atoms embedded into the first layer of Cu(100) surface. We use a combination of molecular dynamic (MD) [3] and kinetic Monte-Carlo (kMC) methods [4].

As result, we’ve got the following conclusions: (i) the formation of compact nanostructures from Co atoms embedded into the first layer of Cu(100) surface without covering with substrate’s atoms can be realized only in the narrow range of temperatures near 400K. (ii) The motion of embedded Co atoms at these temperatures is the result of an intensive diffusion of substrate vacancies. (iii) During the evolution of embedded Co atoms system, in general, zigzag Co structures are formed. Moreover, we’ve investigated the influence of variation of Co atoms concentration and vacancy concentration to the evolution of the system.

References