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Understanding structural modulations in ultrathin Fe films on Cu(001): A systematic approach based on the bulk transition path XIE ZHANG, TILMANN HICKEL, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, Germany, JUTTA ROGAL, Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universitaet Bochum, Bochum, Germany, JOERG NEUGEBAUER, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, Germany — Despite the application of various experimental and theoretical techniques, a proper structure model for the ultrathin Fe films on Cu(001) is missing. This is due to the challenging task to search for possible metastable modulated structures in the high-dimensional configuration space. In this work, we have developed a theoretical approach based on *ab initio* computations to significantly reduce the dimensionality of the configuration space by transferring the insights obtained from our recently identified fcc-bcc transformation path in the bulk with the orientation relationship observed in the ultrathin Fe film experiments. Using this approach, we are able to interpret the complex lattice modulations and surface reconstructions in terms of simple structural motifs, and explain the structural and magnetic features of the experimentally observed distinct regimes in the films. These insights improve our understanding of the fundamental interplay between magnetism and structure in Fe-based materials.

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