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Novel Contributions to Magnetic Anisotropy of Inhomogeneous Materials: Exchange Mediated Magnetic Anisotropy MARKUS EISENBACH, G. MALCOLM STOCKS, BALAZS UJFALUSSY, Oak Ridge National Laboratory, BALAZS GYORFFY, University of Bristol, UK — Calculating and understanding the magnetic behavior of non-homogeneous systems requires careful consideration of the relevant magnetic states. This is especially true in the case of systems that include induced magnetic moments. To study this we consider monatomic magnetic impurities embedded in non-magnetic metals. By performing fully relativistic self consistent calculations for these systems we can investigate the spin orbit coupling effects leading to anisotropies. In contrast to what would be accessible by force theorem calculations, which are useful for systems with robust magnetic moments, this approach allows us to take into account the possibilities of qualitative change in the induced moments. We find that in the case of a monatomic iron impurity in fcc Cu the induced magnetic moments on neighbouring Cu sites align parallel with the Fe moment, whereas for the hard directions some of the induced moments are oriented anti-parallel. This effect, which arises from slight differences in the energies associated with different m quantum numbers, leads to a significant contribution to the magnetic anisotropy due to the resulting exchange energy that can not be captured by a force theorem approach.

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