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Non-collinear magnetism in Permalloy ($Ni_{0.8}Fe_{0.2}$) MARKUS EISENBACH, DON NICHOLSON, G. MALCOLM STOCKS, Oak Ridge National Laboratory — Permalloy is an important material in a wide variety of magnetic systems, most notably in GMR read-heads. However, despite this great interest its properties are not fully understood. For an in depth analysis of important physical properties as e.g. electric transport or magnetic anisotropy a detailed understanding of the distribution of magnetic moments on an atomic level is necessary. Using our first principles Locally Self-consistent Multiple Scattering (LSMS) method we calculate the magnetic ground state structure for a large super-cell model of Permalloy. Our code allows us to solve both the usual non-relativistic Schrödinger equation as well as the fully relativistic Dirac equation and to find the magnitude and direction of the magnetic moments at each atomic site. While the non-relativistic calculation yields a collinear ground state in accordance with previous calculations, we find the ground state for the fully relativistic calculation to be slightly non-collinear. We also investigate the influence of variations in the iron concentration on the distribution of magnetic moments. Research sponsored by DOE-OS and BES-DMSE under contract number DE-AC05-00OR22725 with UT-Battelle LLC. The calculations presented were performed at the Center for Computational Sciences (CCS) at ORNL and at the National Energy Research Scientific Computing Center (NERSC).

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