AB INITIO CALCULATIONS OF THE MAGNETOCRYSTALLINE ANISOTROPY IN $UAuSb_2$ FERROMAGNET

J.A. Morkowski
Institute of Molecular Physics, Polish Academy of Sciences,
ul. M. Smoluchowskiego 17, 60-179 Poznan, Poland

9.7 cm

Magnetic properties of the tetragonal uranium-transition (or noble) metal diantimonides are studied over the last decade (see [1]). Recently details of the electronic structure of $UAuSb_2$ obtained from first-principles calculations and X-ray photoemission spectroscopy were reported [2]. $UAuSb_2$ is a strongly anisotropic ferromagnet below 36 K [1]. The present paper presents results of ab-initio calculations of the magnetocrystalline anisotropy of $UAuSb_2$. The total energy of the unit cell of $UAuSb_2$ was calculated by the full potential LMTO method using the LmtART code (for references and details of computations see [1]). The computations were done for the following orientations of the magnetization vector **M**: [1,0,0], [0,0,1], [0,1,1], [1,1,0] and [1,1,1] in the tetragonal unit cell. The differences of the values of the total energy for various pairs of directions of **M** were fitted by the least-squares procedure to the expression for the magnetocrystalline energy suitable for tetragonal symmetry $E_A = K(\alpha_1^4+\alpha_2^4)+K_2\alpha_3^2$ where $(\alpha_1, \quad \alpha_2, \quad \alpha_3)$ is a unit vector along the direction of magnetization **M**. The calculated anisotropy constants at T=0 are $K = -7.2MJ/m^3, \quad K_2 = -2.9MJ/m^3$. The anisotropy appears to be very strong. The easy axis of magnetization is along [1,0,0].

[1] D. Kaczorowski et al. Phys. Rev. **B58**, 9227 (1998)
[2] J.A. Morkowski et al. J. Alloys Compd. **443**, 20 (2007)

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Corresponding author :
J.A. Morkowski

Address for correspondence :
Institute of Molecular Physics, Polish Academy of Sciences,
ul. M. Smoluchowskiego 17,
60-179 Poznan, Poland

Email address :
jmorkows@ifmpan.poznan.pl