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Simulated thermomagnetic properties of $DyAl_2$, $HoAl_2$ and $ErAl_2$ compounds calculated by atomic matters MFA computation system

We present the results of calculations of magnetic properties of three compounds from Laves phase C15 family: $DyAl_2$, $HoAl_2$ and $ErAl_2$ performed with a new computation system called atomic matters MFA. We compare these results with the recently published results for $TbAl_2$, $GdAl_2$ and $SmAl_2$. The calculation methodology was based on the localized electron approach applied to describe the thermal evolution electronic structure of rare-earth R^{3+} ions over a wide temperature range and to compute magnetocaloric effect (MCE). Thermomagnetic properties were calculated based on the fine electronic structure of $4f^9$, $4f^{10}$ and $4f^{11}$ configurations of the Dy^{3+}, Ho^{3+}, Er^{3+} ions, respectively. Our calculations yield the magnetic moment value and direction; single-crystalline magnetization curves in zero field and external magnetic field applied in various directions of $m(T, B_{ext})$; the 4*f*-electronic components of specific heat $c_{4f}(T, B_{ext})$; and temperature dependence of the magnetic entropy and isothermal entropy change with external magnetic field $-\Delta S(T, B_{ext})$. The cubic CEF parameter values used for $DyAl_2$ calculations are taken from earlier research of A.L. Lima, A.O. Tsokol and recalculated for universal cubic parameters (A^m_n) for the RAl_2 series. Our studies reveal the importance of multipolar charge interactions when describing thermomagnetic properties of real 4*f* electronic systems and the effectiveness of an applied self-consistent molecular field in calculations for magnetic phase transition simulation.

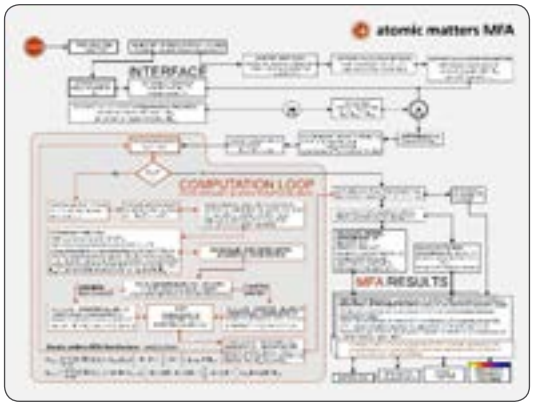

Figure 1: Atomic Matters MFA, calculation algorithm.

Recent Publications

1. Rafał Michalski and Jakub Zygadło (2018) Predictions of thermomagnetic properties of Laves Phase compounds: $TbAl_2$, $GdAl_2$ and $SmAl_2$ performed with atomic matters MFA computation system. Journal of Magnetism and Magnetic Materials 452:415–426.
2. Rafał Michalski, Jakub Zygadło and Marek Karaś (2017) Effective methodology for calculation of magnetic properties of atomic systems in ordered state and around phase transition temperature. WSEAS Transactions on Computers 16:69-75.

3. Rafał Michalski and Jakub Zygadło (2017) Spin and orbital moment compensation in $SmAl_2$. Calculations performed with atomic matters MFA computation system. International Journal of Applied Physics 2:11-17.
4. Rafał Michalski and Jakub Zygadło (2017) Predictions of thermomagnetic properties of $HoAl_2$ and $ErAl_2$ performed with atomic matters MFA computation system. WSEAS Transactions on Circuits and Systems 16:22-34.
5. Rafał Michalski and Jakub Zygadło (2017) Thermomagnetic properties of $DyAl_2$ single crystal, calculated by atomic matters MFA computation system. WSEAS Transactions on Applied and Theoretical Mechanics 12:69-77.

Biography

Rafał Michalski graduated in 1996 from the Pedagogical of University Krakow, Poland in the department of Physics, Mathematics and Computer science. He worked in the Institute of Physics and Computer Science as an Assistant Professor (1996-2001) and then in 2001 he gained a PhD in physics in the department of Nuclear Physics and Solid State Physics at Krakow University of Mining and Metallurgy (AGH). Subsequently, he became an associate professor. His PhD Thesis was "*Calculations of the thermal evolution properties of 4f-electron compounds with the use of the self-consistent methods*". In 2001, dr R. Michalski become a leader of a Polish Scientific Research Committee project (no 1463/P03/2002/22) entitled "The Effects of crystalline symmetry in ThCr2Si2 type Rare Earth compounds". The project ended 31.12.2002. Simultaneously, he worked at the Center for Solid State Physics with prof R.J. Radwański (1996-2006) and published around 30 papers about Crystal Field (CEF) and spin-orbit coupling (SO) effects in materials. At the same time, R. Michalski created two free access computing packages: BIREC (Basic Interactions in Rare-Earth Compounds) and CEF for 3d ions (Crystal Electric Field for 3d ions) to simulate the fine electronic structure and examine the consequences of such a structure on properties of solids as a function of temperature. In 2006-2011 R. Michalski cooperated with a consulting company providing services for industry research projects and deployment of innovative technologies. During this time he invented some commercial technologies protected by 5 patent applications in the EU and the USA. In 2012, he set up and worked for a Light Source Photometry Laboratory for MILOO Electronics. In 2008, R. Michalski started his own commercial scientific activity and developed a project co-financed by European Union resources of the regional development fund (UDA-POIG.01.04.00-12-069/10-00) entitled: "Creation of tools for comprehensive analysis of magnetic properties of elements". The result of this project was an application called Atomic Matters, which simulates the influence of crystal lattice charge surroundings on any atom/ion from the periodic table (www.atomicmatters.eu). Atomic Matters is designed to calculate, simulate and visualize the most relevant properties of materials which are determined by the fine electronic structure of contained ions or atoms in defined conditions. After completing this project, R. Michalski lead a team of programmers in the creation of ATOMIC MATTERS MFA software. ATOMIC MATTERS MFA is an extension of Atomic Matters for magnetic phase transition simulation by self-consistent calculations according to Mean Field Approximation methodology. The synergy of both applications makes it possible to predict the macroscopic properties of materials in user-defined temperature region by using the physical properties of atomic electron systems under the influence of an external magnetic field. The visual form of the results of calculations (including full 3D interactive CEF potential visualization), intuitive interface and tools, and comparative data makes the application extremely efficient and easy for new users. The premiere presentation of ATOMIC MATTERS MFA software was at Thermag VII, the Seventh IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature, Torino Italy, 11-14 September 2016. R. Michalski has managed and participated in about 20 scientific projects. He is has authored more than 40 articles published in international journals and conference proceedings.

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