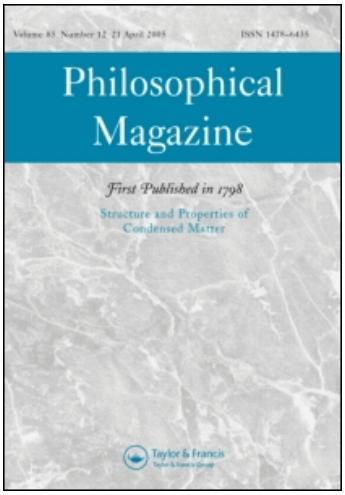

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The James Clerk Maxwell Young Writer's Prize *Nurturing tomorrow's researchers in Physics and Materials Science*

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EDITORIAL

The James Clerk Maxwell Young Writer's Prize
Nurturing tomorrow's researchers in Physics and Materials Science

We are pleased to announce the winner of the The James Clerk Maxwell Young Writers Prize for 2009. **Dr Giovanni Bonny** of Nuclear Materials Science Institute, SCK-CEN, Belgium, won the first prize of $1,000 with his paper 'Fitting interatomic potentials consistent with thermodynamics: Fe, Cu, Ni and their alloys'. There were three runners-up whose papers were awarded the distinction of being highly commended.

> Dr Bonny writes: "*I feel very honoured to have received this prestigious prize. It is a great feeling to know that my PhD. work is recognised and appreciated by the scientific community. I am now more than ever determined to continue to perform quality research. To conclude, I would like to emphasise that this work was a team effort and therefore I take this opportunity to acknowledge my co-authors, Drs Lorenzo Malerba and Roberto Pasianot, for their guidance and support. Another word of gratitude goes to my collaborator and friend, Dr Dmitry Terentyev; and to my eternal inspiration and partner in life, Eva Laura Schor.*"

Giovanni Bonny completed his PhD. at Ghent University (Belgium) in June 2009. His PhD. dissertation focusses on the development of interatomic potentials for large-scale atomistic simulations. With such simulations he aims to get a deeper understanding of the mechanisms governing materials degradation under irradiation. Currently Giovanni is pursuing a post-doctoral fellowship at SCK-CEN (Belgium).

Publication details and outlines of the contents of the papers of the winner and the three runners-up are given below.

Winning Entry

Giovanni Bonny
Nuclear Materials Science Institute, SCK-CEN, Belgium

Fitting interatomic potentials consistent with thermodynamics: Fe, Cu, Ni and their alloys

G. Bonny, R.C. Pasianot & L. Malerba
Philosophical Magazine Volume 89 Issue 34 Pages 3451–3464.

Outline

The paper focusses on two fitting techniques to develop interatomic potentials. In computational materials science, large-scale atomistic methods hinge on an interatomic potential to describe the material properties. In alloys, besides a proper description of problem-specific properties, a reasonable reproduction of the experimental phase diagram by the potential is essential. In this framework, we

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developed two complementary methods to fit interatomic potentials to the thermodynamic properties of solid phases in alloys. The first method involves the zero-Kelvin phase diagram and makes use of the concept of the configuration polyhedron. With this method some desired intermetallic compounds can be stabilised as true ground states of the system. The second method involves the phase stability at finite temperature and is based on the cluster variation method. With this method it is possible to closely fit experimentally observed phase boundaries. As an example of both techniques, we applied them to the Fe-Cu, Fe-Ni and Cu-Ni systems.

Highly Commended Entries

Ignacio A. Figueroa
Sheffield University, UK

High glass formability for Cu-Hf-Ti alloys with small additions of Y and Si

I.A. Figueroa, H.A. Davies & I. Todd
Philosophical Magazine Volume 89 Issue 27 Pages 2355–2368.

Outline

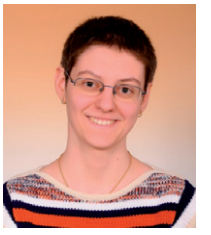
This paper reports and discusses the effects of *small* substitutions of Si and Y for Cu on the glass forming ability (GFA) of the ternary alloy Cu55Hf25Ti20. Substitutions of only 0.5 at.% Si and 0.3 at.% Y resulted in substantial increases in the diameters of fully glassy rods from 4mm for the base alloy up to 7 and 6.5mm, respectively. It is proposed that these increases are related to the effects of Si and Y in either removing or strongly reducing the number density of heterogeneous nucleating particles of TiO2, Ti2O3 and/or HfO2 in the molten Cu55Hf25Ti20 alloy, prior to solidification. (The negative molar heats of formation of these three oxides increase in the sequence TiO2, HfO2, Ti2O3, though we have no information about their relative magnitudes in an environment of liquid Cu55Hf25Ti20 alloy). In the case of Y, it is proposed that the dopant addition would reduce the Hf and/or Ti dioxides to form the chemically more stable Y2O3. There is evidence in the literature which suggests that the contact angle between a CuTi based alloy and Y2O3 may be slightly too large for this oxide to act as a heterogeneous nucleating agent to the extent of influencing the overall nucleation behaviour, i.e. the nucleation is then dominated by the homogeneous process. In the case of the Si addition, it is suggested that the HfO2 particles combine with Si to form the thermodynamically more stable HfSiO4 phase. This phase is a strong network former (probably, in this case, containing Cu and Ti as network modifiers) and, as for other silicates, would be expected to solidify to *glassy* phase particles prior to the quenching of the liquid alloy. Thus, the potency of the pre-existing crystalline Hf (or Ti) oxides as heterogeneous nucleating agents would be nullified by the Si addition. For concentrations beyond 0.5% Si and 0.3% Y, the effects of these solutes on the GFA become saturated, as the pre-existing crystalline oxides are consumed, and thus the critical rod diameters for a fully glassy

phase then diminish, consistent with the *intrinsic* effects of these and several other solutes on the GFA of this and similar ternary Cu-Ti-based alloys.

Réka Trencsényi
University of Debrecen, Hungary

Correlation and confinement induced itinerant ferromagnetism in chain structures

Réka Trencsényi, Endre Kovács & Zsolt Gulácsi
Philosophical Magazine Volume 89 Issue 22 Pages 1953–1974.



Outline

Using a positive semidefinite operator technique we deduce exact ground states for a zig-zag hexagon chain described by a non-integrable Hubbard model with on-site repulsion. Flat bands are not present in the bare band structure, and the operators introducing the electrons into the ground state, are all extended operators and confined in the quasi-1D chain structure of the system. Consequently, by increasing the number of carriers, these operators become connected, i.e. touch each other on several lattice sites. Hence the spin projection of the carriers becomes correlated in order to minimise the ground-state energy by reducing as much as possible the double occupancy, leading to a ferromagnetic ground state. This result demonstrates in exact terms in a many-body frame that previous conjectures made at two-particle level [Phys. Rev. Lett. 93, 146405, (2004)] that the Coulomb interaction is expected to stabilise correlated magnetic ground states in acenes, are clearly viable, and open up new directions in the search for routes in obtaining organic ferromagnetism. Due to the itinerant nature of the obtained ferromagnetic ground state which emerges as a joint effect of correlations and confinement, the systems under discussion may also have direct application possibilities in spintronics.

Tao Xu
Georgia Institute of Technology, USA

Topological and statistical properties of a constrained Voronoi tessellation

T. Xu & M. Li
Philosophical Magazine Volume 89 Issue 4 Pages 349–374.

Outline

In this article, we present an extended version of the Voronoi tessellation method that partitions the space with certain constraints commonly encountered in either experimental measurements or theoretical models, such as cell volume or size distribution. The topological and statistical properties of tessellated Voronoi cells are calculated in several model systems with cell volumes obeying lognormal and bimodal distributions. Systematic changes in the topological properties and deviations from some established topological relations, such as Lewis rule

and Aboav–Weaire Law, are observed as the parameters in the constraints vary. The most significant contribution of this method is to generate realistic digital microstructures with any desired topological and geometrical properties for theoretical simulation and characterisation in poly- and nano-crystalline materials.

There is free access to these three papers until the end of July 2011 via the James Clerk Maxwell Young Writers Prize website: www.tandf.co.uk/journals/authors/tphm-tphl-prize.asp.

If you are a young writer who has authored or co-authored a paper in *Philosophical Magazine* or *Philosophical Magazine Letters* during 2010, or intends to do so, you could be in the running for next year's prize. To be eligible you should be a PhD. student at the time of writing the paper or have completed your PhD. within the two previous years. You will also need to be nominated by your supervisor or senior author of the paper. The nomination form and terms and conditions can be found at http://www.tandf.co.uk/journals/authors/tphm-prize.doc.

We look forward to receiving entries for the 2010 prize, the closing date for which is 31st December 2010.

Professor E.A. Davis
Coordinating Editor